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Large-Eddy Simulation

Guidelines for its application to planetary boundary layer research

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Edited by
J. C. Wyngaard

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LARGE-EDDY SIMULATION:
GUIDELINES FOR ITS APPLICATION
TO PLANETARY BOUNDARY LAYER RESEARCH

Final Report

from

The Working Group on Large-Eddy Simulation

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After a review of the current status of turbulence and diffusion modeling in the planetary boundary layer (PBL) and engineering fluid mechanics, the Working Group on Large Eddy Simulation (LES) concluded that inherent uncertainty is a major complication to atmospheric experiments and modeling and that data bases for future models of PBL are unlikely to be derived from field experiments. The roles of LES in quantifying inherent uncertainty and in providing appropriate data bases for analysis are discussed. Long range guidelines for →

PBL research using LES are presented (i) for the technical components of a program--turbulence theory, computational problems and requirements, physical and numerical experiments and transfer of technology to less complex models-- and (ii) for the management program to stimulate research in envrionmental fluid mechanics.

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PREFACE

On June 15 and 16, 1983, the U.S. Army Research Office (ARO) convened about 20 experts in a workshop with the theme "Aerosol Dispersion in the Atmospheric Surface Layer" (Bach, 1984). This workshop brought forth the recommendation that ARO establish a working group to investigate "large-eddy simulation," or three-dimensional, time-dependent, fine-mesh numerical modeling of turbulent flows. Known as LES in the engineering community, it had actually been pioneered by J. Deardorff of the National Center for Atmospheric Research (NCAR) in the late 1960s. The ARO workshop recommended further that this working group prepare long-range priorities for introducing large-eddy simulation (LES) models into the Army research program.

ARO accepted these recommendations and assigned Walter D. Bach, Jr., a meteorologist in the ARO Geosciences Division, the responsibility for their implementation. He established as objectives for the working group:

A. To study the feasibility of using LES as a surrogate method of obtaining the temporal and spatial distributions of mass, momentum, heat, and moisture in the atmospheric boundary layer, subject to given initial and boundary conditions and, using these distributions, to examine the behavior of gases and aerosols within the modeled volume; and

B. To recommend a course of action for implementing LES techniques that are feasible and appropriate for the Army's needs in basic research on atmospheric dispersion of gases and aerosol.

In October 1983, I agreed to head the Working Group on Large-Eddy Simulation. I chose as members Dr. Stephen Burk, Naval Environmental Prediction and Research Facility, Monterey; Prof. William Cotton, Department of Atmospheric Science, Colorado State University; Prof. Joel Ferziger, Department of Mechanical Engineering, Stanford University; Dr. Steven Hanna, Environmental Research and Technology, Inc., Concord, Massachusetts; Dr. Parvis Moin, NASA Ames Research Center; Mr. William Ohmstede, Atmospheric Sciences Laboratory, White Sands; and Dr. Jeffrey Weil, Martin Marietta Corp., Baltimore. Walter D. Bach, Jr. also participated fully in our deliberations.

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Our working group met in Boulder, Colorado, on Dec. 5 and 6, 1983, and on Feb. 6, 1984. Each member also spent a good deal of individual time in researching and compiling his contribution, which I have tried to blend into a unified document.

On behalf of the working group I want to thank Walter D. Bach, Jr. who made it possible for us to participate in this most rewarding project, and Shirley Michaels of Michaels Communications, who splendidly administered the Working Group on Large-Eddy Simulation and expertly produced this report, our final product.

John C. Wyngaard
Boulder, Colorado
August 1984

EXECUTIVE SUMMARY

The planetary boundary layer (PBL) has numerous challenging but complicating features. Its physics are more intricate than those of many other turbulent flows; buoyancy, phase-change, and radiative effects can complicate the usual turbulence dynamics. Another challenge is its "inherent uncertainty," the inevitable difference between its most likely (i.e., ensemble-average) state and its actual behavior over a finite time interval. Inherent uncertainty is a major obstacle to the application of PBL models to real problems. It also greatly increases the difficulty and expense of direct measurements in the PBL, making it necessary to assemble vast quantities of data in order to produce reliable statistics.

There are two broad approaches to the numerical modeling of the PBL—one based on ensemble averaging, the other on volume averaging. The ensemble-average approach has traditionally used eddy-diffusivity closure, which began to give way in the 1970s to second-order closure. Each has strong limitations, however, and simpler models using integral closures (e.g., the Gaussian-plume model for turbulent dispersion) also enjoy wide use. Three-dimensional, time-dependent, fine-mesh, volume-average modeling (large-eddy simulation, or LES) can in principle give far more powerful predictions than these other methods, but is also far more expensive.

The engineering fluid mechanics community has invested considerable resources over the past decade in developing LES for shear-flow applications. Today it is a viable complement to experiment in both fundamental and applied turbulence research. Its growing popularity reflects both its promise of realistic answers to difficult problems and the continuing rapid decline in computing costs.

The roots of the LES technique actually lie in meteorology; the first engineering application of LES was Deardorff's simulation of turbulent channel flow, which was carried out at the National Center for Atmospheric Research in the late 1960s. Today LES is used in small-scale-meteorology problems ranging from PBL structure to severe-storm dynamics.

We drew three major conclusions from our assessment of the current status of PBL research:

1. Inherent uncertainty is a major complication, strongly influencing both experiment and modeling. There have been few attempts to generalize models to include prediction of inherent uncertainty; in general this remains a challenge for the future. Meeting this challenge will require a broader, more reliable PBL data base than now exists.

2. Because of their cost, difficulty, and limitations, field experiments cannot be expected to provide the improved PBL data base necessary for the next generation of models. However, this data base would benefit greatly from measurements in carefully designed laboratory experiments which simulate certain aspects of the PBL.

3. LES experiments also have the potential of contributing substantially to this data base through "field programs" on the computer. Although LES has some limitations in PBL applications (e.g., loss of eddies larger than the domain size, poor resolution near bottom and top, difficulties with boundary conditions), the advances which we expect in supercomputers over the next several years should ease these somewhat. LES experiments also have unique advantages, such as allowing the experimenter to control individual variables in order to study their effect on the flow.

In view of these findings and considering the recent history of LES in both engineering fluid mechanics and small-scale meteorology, we perceived two broad roles for LES in future PBL research:

1. Studying the sources and physics of inherent uncertainty and quantifying it for applications, particularly in turbulent dispersion.

2. Generating data bases for developing profiles for integral models; for studying dynamics; for developing parameterizations for higher-order-closure models and for subgrid-scale processes in meteorological models; and in designing and simulating PBL experiments.

We established general guidelines for the development of LES models for the planetary boundary layer in order that investments in LES research can provide optimum returns. We recommend a development program having

theoretical, computational, experimental, and technology-transfer components. Key challenges here include:

- Theory--subgrid-scale parameterization (including subgrid-scale dispersion) in LES models; optimum choice of modes; boundary conditions; numerical techniques for dispersion applications; inclusion of mesoscale-eddy effects.
- Computation--the use of full turbulence simulation to stimulate LES development.
- Experiment--the use of both atmospheric and laboratory data to test LES predictions.
- Technology transfer--quantifying inherent uncertainty; developing higher-order-closure parameterizations; developing subgrid-scale parameterizations for larger-scale meteorological models.

Supercomputers are revolutionizing the entire field of nonlinear dynamics. Their most direct and powerful application to small-scale meteorology is, in our view, in LES. The impacts of LES to date, while substantial, could be dwarfed by those over the next decade. An optimum response to this opportunity will require the participation of a broad group of individuals and institutions, but will, we believe, bring great rewards.

CHAPTER ONE
INTRODUCTION

In examining the feasibility of three-dimensional, time-dependent, fine-mesh numerical modeling (large-eddy simulation) of the lower atmosphere, we identified several topics that we felt were pivotal and, hence, deserved careful exposition in this report.

We recognized that the planetary boundary layer (PBL) has numerous challenging but complicating features. These include what is called "inherent uncertainty," the inevitable difference between its most likely (i.e., ensemble-average) state and its actual behavior over a finite time interval. Inherent uncertainty has come to be recognized as a major complication in the application of PBL models to real problems. The physics of the PBL are also more intricate than those of many other turbulent flows; buoyancy, phase-change, and radiative effects can all add complications to the usual turbulence dynamics. Consequently, we agreed that an optimum approach to PBL research would combine the strengths of observational studies (both in the laboratory and outdoors), theoretical work, and numerical modeling. We have devoted Chapter Two to these issues.

We identified several contemporary approaches to the numerical modeling of the PBL and, in particular, of diffusion within it. The traditional closure for ensemble-averaged equations, eddy diffusivity, began to give way somewhat in the 1970s to second-order closure. Each has a range of applicability, but since neither represents a fundamental solution to the closure problem, neither can be a general-purpose tool. Integral models, such as the Gaussian-plume diffusion model well-known in regulatory applications, are simple and cheap; however, they do not address some important questions such as short-term behavior. Three-dimensional, time-dependent, fine-mesh modeling (LES) can in principle give far more powerful predictions than other approaches, but is also far more expensive. We devote Chapter Three to an examination of these modeling techniques.

The engineering fluid mechanics community has invested considerable resources in developing LES over the past decade, and we felt it important to review the progress they have made. We do this in Chapter Four, and conclude that chapter with our view of the future prospects for LES in engineering flows. We include as an Appendix the paper, "Numerical Simulation of Turbulent Flows," by Robert S. Rogallo and Parviz Moin, which appeared originally in Annual Review of Fluid Mechanics, v. 16, and which describes the current state of the art of LES in engineering.

The roots of the LES technique lie in meteorology, thanks to pioneering work by D.K. Lilly, J.W. Deardorff, and others. Ironically, LES is underutilized today in small-scale meteorology, in our view, although it is being fruitfully applied to studies ranging from PBL structure to severe-storm dynamics. We survey these meteorological applications in Chapter Five.

We perceived two broad and important roles for LES in the planetary boundary layer research of the future. It offers perhaps our best hope for quantifying inherent uncertainty, which has recently emerged as an important issue in diffusion modeling. Further, it has vast potential for building data bases on PBL structure and processes; this is very important in view of the increasing difficulty and expense of direct measurements. We cover these issues in Chapter Six.

Chapters Two through Six thus provide a comprehensive assessment of the LES technique in the broad context of research challenges in the atmospheric boundary layer. In Chapter Seven, we discuss our recommendations for an LES-based PBL research program. We have avoided being overly specific, preferring to leave a good deal to the creativity of the investigators; however, we have presented our views on high-payoff areas which deserve early attention.

CHAPTER TWO

THE CHALLENGES AND COMPLICATIONS OF PBL RESEARCH

In this chapter we will first discuss those features which distinguish the PBL from other turbulent flows. These include, most importantly, buoyancy, phase-change, and terrain effects. Next, we will discuss another feature, inherent uncertainty, which is very important in numerical modeling and observational studies of the PBL. Then we will cover methods of attack. At the present time, these include experiment, both in the laboratory and outdoors, and numerical modeling. Finally, we will discuss those features of the PBL which are particularly relevant to dispersion problems.

2.1 PBL Physics

Unlike most turbulent flows in engineering, in which the turbulence is produced by mean velocity shear, the PBL tends to be dominated by buoyancy effects. With clear skies at night over land, stable stratification develops in the lowest few tens to few hundreds of meters, suppressing the turbulence levels and keeping eddy sizes small. As a result, turbulent dispersion is greatly reduced. By contrast, surface heating in the daytime tends to produce a convectively driven PBL whose eddies are much larger, more intense, and consequently more dispersive. Thus, the turbulence dynamics of the stable and unstable PBLs are quite different, and also different from those of engineering shear flows.

Thermal effects are also pronounced on the next larger scales, from a few to a few tens of kilometers, where a horizontal temperature gradient hydrostatically creates a vertical change in the horizontal pressure gradient. For example, temperature gradients of a few K per 100 kilometers (which are common after frontal passages, for example) can change the horizontal pressure gradient substantially in the lowest 1000 m, and this can lead to large mean wind shears in the PBL.

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Over land, the earth's surface is apt to have considerable "texture"--
e.g., spatially varying albedo, surface roughness, and elevation. In
conjunction with heating or cooling, this can lead to "standing" eddies of
substantial magnitude. Land-sea breezes and the diurnal upslope/downslope
cycle over sloping terrain are good examples. These can have very strong
influences on local diffusion patterns.

The PBL transports water vapor which forms clouds when lifted above the
condensation level. The associated energy release can generate large vertical
velocities as well, and can lead to large-scale circulation patterns which
strongly influence the structure of the PBL below.

These are a few of the features which complicate the PBL. In the opinion
of the committee, they will prevent its early understanding at the level that
we now enjoy for canonical laboratory flows, such as the jet, wake, and mixing
layer.

2.2 Inherent Uncertainty

A dominant trait of the PBL is its spatial and temporal variability.
Although this variability is common to all turbulent flows, it is more
pronounced in the PBL than in typical engineering flows (e.g., in pipes)
because of the greater range of space and time scales involved.

Mathematical modeling of turbulent flows in general and the PBL in
particular becomes tractable only when the governing equations are averaged
over time, space, or an ensemble of realizations. Hence, any comparison of
model predictions with (error-free) observations under supposedly the "same"
meteorological conditions is apt to reveal deviations between the two. These
deviations will have a mean, or bias, and a variance. The bias is due solely
to internal model errors (e.g., physics, parameterizations, coding), whereas
the variance is due to three factors: 1) uncertainties in model input
variables, 2) internal model errors, and 3) inherent uncertainty (see Fox,
1984; Venkatram, 1982). The bias can be reduced by reducing internal model
errors, but the variance cannot.

The inherent uncertainty is typically a major component of the
variance. It arises because the details of the initial and boundary
conditions describing the flow are not the same in individual realizations,

even though the gross conditions (e.g., mean wind speed, surface heat flux) describing the ensemble are. Clearly, an endless number of different initial and boundary conditions (on a fine scale) could be associated with the same gross conditions. The magnitude of the inherent uncertainty also depends on the number of physical parameters entering the model. The ensemble is defined differently as this number changes. In any event, we should expect departures of individual realizations from ensemble averages.

Inherent uncertainty in a property f is defined by $\sigma^2 = \langle(\overline{f - \langle f \rangle})^2\rangle$, where the overbar denotes a time or space average and the brackets denote an ensemble average. If the random process is stationary and ergodic, σ^2 is given by

$$\sigma^2 = \frac{2\langle f'^2 \rangle \tau}{T} , \qquad (1.1)$$

provided that $T \gg \tau$, where T is the averaging time, τ is the integral time scale of the process, which we assume exists, and $\langle f'^2 \rangle$ is the ensemble variance (Lumley and Panofsky, 1964). Thus, inherent uncertainty depends on the particular process, through $\langle f'^2 \rangle$ and τ, and on averaging time.

Basic to an ensemble is the requirement that individual realizations be obtained under the conditions which are understood to define the experiment. In model verification the definition of these conditions is of paramount importance (Chatwin, 1982; Venkatram, 1984a); it would be given by the model inputs. Thus, we can see that inherent uncertainty is also model dependent.

Why is inherent uncertainty so important? The principal reason is that for many PBL variables the ratio of σ to the ensemble mean $\langle f \rangle$ is of order 1 for the short averaging times (~1 hour) typically of interest. Wyngaard (1983) has discussed $\sigma/\langle f \rangle$ for some PBL properties and Venkatram (1979) considers it for ground-level concentrations downwind of elevated stacks. Worst-case examples are humidity fluctuations, especially in a cloud-topped PBL, and ground-level concentration variability downwind of an elevated point source. In the latter case, the geometric standard deviation of hourly averaged concentrations is about 2 along the plume axis during convective conditions (Weil and Brower, 1984).

Thus, it is necessary to know σ, the inherent uncertainty, to describe fully the state of the PBL, and dispersing plumes within it, for short

averaging times. Specifically, one needs it to predict the frequency of occurrence of certain high concentration events in plumes, e.g., the flammability, or toxicity, limits in dense gas releases (Chatwin, 1982). In addition, inherent uncertainty is a key factor in model verification. One thing is clear: when $\sigma/\langle f \rangle$ is large, simply describing the PBL in terms of ensemble means is grossly inadequate, because many individual realizations will have properties far removed from the mean.

Inherent uncertainty in dispersion modeling is closely related to the concentration fluctuations in plumes. The latter subject has a history dating back to at least 1959, when Gifford's meandering plume model appeared.

Concentration fluctuations in plumes are a strong function of the source and plume geometry as well as the averaging time. On the basis of the models of Gifford (1959), Sawford (1983), and Venkatram (1984b), as well as field observations and laboratory experiments (Fackrell and Robins, 1982; Deardorff and Willis, 1984), we know that for an elevated point source, lateral and vertical-plume meandering by large eddies is the principal cause of the large concentration fluctuations along the mean plume axis. These large fluctuations ($\sigma_c/\langle c \rangle > 1$) occur at all distances from the source because of the presence of lateral energy at all scales in the atmosphere.

Simple models have been advanced to predict concentration fluctuations for a variety of situations (see Hanna, 1984). For example, Csanady (1967) and Netterville (1979) developed K-models to predict the ensemble concentration variance, $\langle c'^2 \rangle$, due to relative turbulence alone. Empirical Gaussian models for the same purpose have been put forth by Wilson et al. (1982). The Gifford (1959) model can be used to estimate the fluctuations due to meandering, provided that one can estimate the dimension of the "instantaneous" plume and the characteristics of the lateral turbulence. Venkatram (1984b) has developed a model for fluctuations of hourly averaged concentrations about ensemble means based on the probability density function of vertical and lateral turbulence velocities, specifically for elevated sources.

In a computer-intensive numerical approach, Durbin (1980) and Sawford (1983) used Lagrangian statistical models to predict the ensemble concentration variance due to meandering as well as relative turbulence in neutral boundary layer flows. These models require information about the turbulence as one follows the plume.
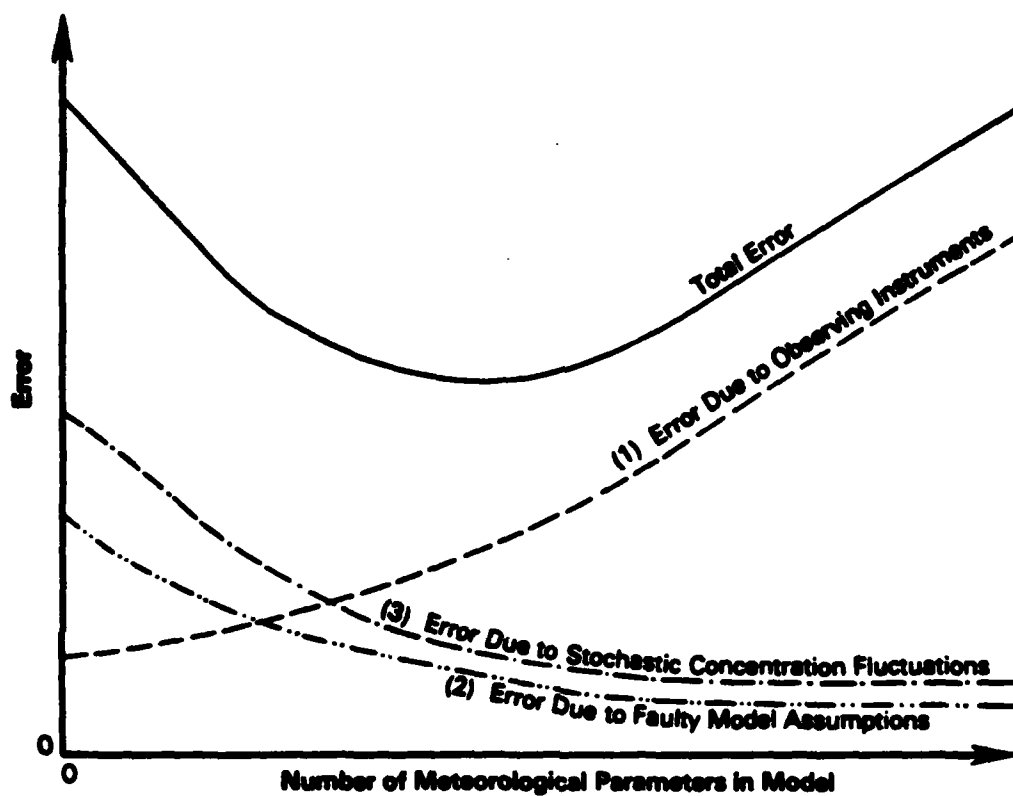
Figure 1. An example of the variation of total model error with number of meteorological parameters. The finite value of component (1) at zero is due to errors in the instrument observing the parameter being predicted.

Once methods are available to estimate concentration fluctuations and, hence, inherent uncertainty for certain classes of models, it might be possible to determine the type of model that would give minimum total error in a given application. As shown in Figure 1, if errors in observing instruments are large, a model with many input parameters could give a larger total error than a model with fewer parameters. Hanna (1975) suggested that this is why simple integral models can predict urban air quality as reliably as much more complex, three-dimensional, time-dependent, gradient-transport models. The complex model might contain much better physics, but requires a set of input data from often poorly sited and maintained instruments.

In summary, we find that inherent uncertainty is increasingly being recognized as an important aspect of boundary-layer meteorology. It is particularly important in dispersion applications, where it is central to the taking of observations and the design of experiments, and to numerical prediction and model verification.

2.3 Laboratory Experiments

Perhaps surprisingly, laboratory experiments offer a valuable and attractive means of investigating flow structure and diffusion in the PBL. Their main advantage is the opportunity they provide for studying a particular phenomenon in isolation and over a range of controlled conditions. They are probably most useful as a complement to other forms of PBL research (e.g., numerical modeling and field observations), but sometimes they offer the only practical means of studying a problem (e.g., wake flows and diffusion).

In the following brief survey, we highlight some laboratory experiments which have made important contributions toward our knowledge of the mean and turbulent structure of the PBL and of diffusion within it. The typical facilities used are wind tunnels, water channels (circulating water or tow tanks), and water convection tanks (no mean flow).

a. PBL structure

The general requirements for similarity between laboratory and full-scale flows are addressed in several articles (e.g., Cermak, 1971, 1975; Snyder, 1972). For problems in which Coriolis effects are not simulated, the principal requirements are typically the matching of a Froude or bulk

Richardson number (i.e., buoyancy force/inertial force) between model and prototype, and the maintenance of a model Reynolds number above some critical value.

Surface layer. The surface layer, that region where surface friction effects are important, can be defined as $z < |L|$, where z is the height above the surface, and L is the Monin-Obukhov (MO) length (Lumley and Panofsky, 1964). In the limit of neutral stratification ($L \rightarrow \infty$), it can be defined as the region where the mean wind follows the logarithmic wind profile (typically $z < 100$ m).

The surface layer was probably the first and most explored region of the PBL in laboratory experiments, with most work confined to wind tunnels, as summarized by Cermak (1971, 1975) and Snyder (1981). Cermak's (1975) review, as well as the experiments by Arya and Plate (1969) and Rey et al. (1979), demonstrate that wind tunnels can simulate the mean wind and temperature profiles. The velocity variances in the tunnel simulations also agree fairly well with the field observations. However, the tunnel simulations are limited to slight departures from neutral stratification ($|z/L| < 0.3$).

Panofsky et al. (1977) showed that horizontal velocity variances in the surface layer depend on the mixed layer depth z_i and, hence, on the large convective circulations below z_i. This means that to simulate properly the horizontal velocity variances in the surface layer, one is required to model a capping inversion layer and the large-scale convection. This remains a challenge for laboratory experimenters.

Canopy Layer. The canopy layer lies between the ground and the top of the surface roughness (crops, trees, etc.); in this layer biologically important processes occur and surface fluxes of heat, moisture, and momentum originate. The upper part of the canopy and the lower part of the surface layer form a transition region called the "roughness sublayer."

Raupach and Thom (1981) give an extensive review of canopy turbulence, including many of the important contributions made by wind-tunnel simulations. Such simulations, which typically have been conducted for neutral flow, have benefited our understanding in at least three ways. First, they have provided details on how the flux-gradient relationships in the roughness sublayer depart from the well-established ones in the surface layer (Mulhearn and Finnigan, 1978). Second, they have shown that the turbulence
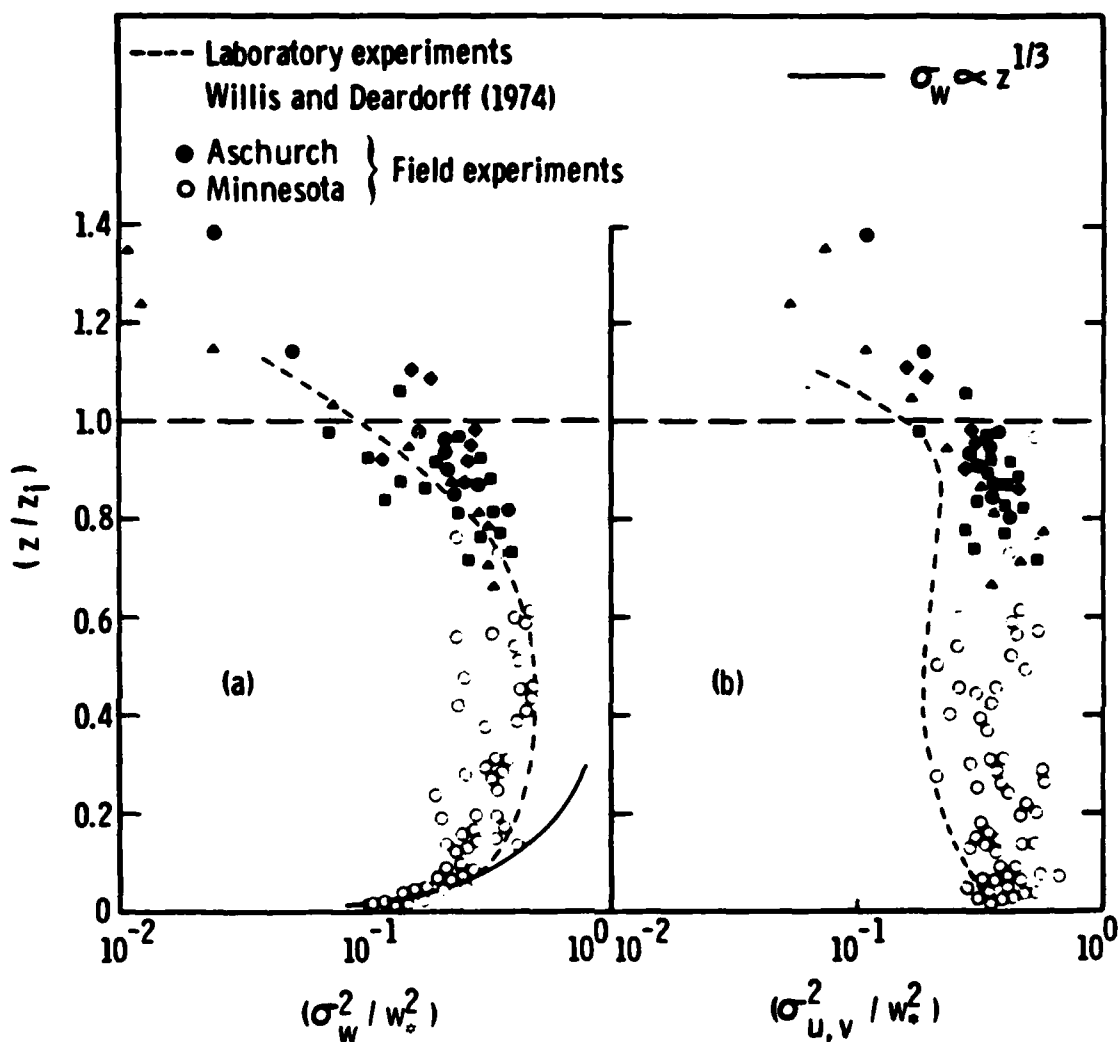
Figure 2. Comparison between field and laboratory measurements of the vertical and horizontal velocity variances in the convective boundary layer (after Caughey and Palmer, 1979). a) Vertical velocity variance, σ_w^2, nondimensionalized by w_*^2, where w_* is the convective velocity scale. Solid line is the free convection prediction: $(\sigma_w/w_*)^2 = 1.8 (z/z_i)^{2/3}$. b) Average of horizontal velocity variances, $\sigma_{u,v}^2$ nondimensionalized by w_*^2. Dashed lines represent the average of S1 and S2 cases in Willis and Deardorff (1974).

spectra and cospectra within the roughness sublayer are height-dependent (relative to the displacement height), whereas they are not in the canopy (Seginer et al., 1976), in agreement with field data. Third, they have helped to demonstrate the importance of turbulent transport in the canopy by organized structures above, and the inapplicability of local diffusion theory within, the canopy (Raupach and Thom, 1981).

We see three areas where further laboratory experiments could be of particular benefit here. The first is the behavior of the flux-gradient relationships for heat and moisture in the canopy and roughness sublayer. The second is turbulent transport of heat, moisture, and momentum by organized structures. The third is the effect of waving plants on the mean and turbulent wind fields (Finnigan and Mulhearn, 1978).

Convective Boundary Layer. One of the triumphs of PBL-oriented laboratory experiments was the simulation of the convective boundary layer (CBL) by Willis and Deardorff (1974). These simulations, whose results have been applied to diffusion as well as to PBL structure, were conducted in a water-filled, free-convection tank, and were motivated by Deardorff's (1972) numerical modeling, which suggested that PBL turbulence properties above the surface layer were independent of surface friction.

Three main aspects of the CBL have been explored with the convection tank. The first was the time evolution of the mean temperature and heat flux profiles (Willis and Deardorff, 1974; Heidt, 1977), which were found to follow the same trends as their atmospheric counterparts. The second was the vertical profile of the velocity variances. Caughey and Palmer (1979) showed that the laboratory vertical component agreed well with field data (Figure 2), but that the horizontal components were about 50% too small, probably due to the small aspect ratio (width/height; ~ 2 to 5) of the tank. The third was the entrainment of stable air at the CBL top. Experimental results from a tank investigation (Deardorff et al., 1980) were used to develop entrainment parameterizations which would be quite difficult to achieve directly from the atmosphere.

Extensions of these experiments would be extremely beneficial to our current understanding of CBL structure. Experiments in a tank of much greater aspect ratio (say 30) would show whether larger horizontal eddies appear with increased horizontal velocity variance. It would be useful to know what aspect ratio gives horizontal variances matching those in the atmosphere.

Another extension is the investigation of baroclinic effects on the mean and turbulence structure; this is especially important for mesoscale modeling. Baroclinicity could be explored in two ways: (1) by using a tank with a slightly sloped bottom and perhaps rectangular rather than square horizontal cross section (Deardorff, personal communication) and (2) by using a tank with nonhomogeneous heat flux to simulate, for example, land/water interfaces.

A third problem worthy of study is the nature of the organized turbulence structure as the stability approaches neutral conditions, say $0 < -z_i/L < 2$, i.e., when surface friction cannot be ignored. Evidence suggests that here the random convective cell structure typical of very unstable conditions changes to one of roll vortex nature (Deardorff, 1982). This investigation would require an experimental facility capable of producing surface shear as well as convection; shear could be produced either by flow of the working fluid over a rough surface or by moving the rough surface (e.g., a moving belt) through the fluid.

Finally, we would encourage further investigation of the entrainment process at the top of the CBL, especially when mixing may be driven by several mechanisms operating simultaneously—convection, surface stress, and velocity shear at the CBL top. Again, a different facility would be necessary to study convectively driven mixing in addition to one of these other mechanisms.

Stable Boundary Layer. Laboratory experiments have been conducted to explore turbulence in several types of stably stratified flows: behind grids (Dickey and Mellor, 1980), in shear layers (e.g., Thorpe, 1973; Lin and Pao, 1979), and in the weakly stable surface layer. However, practically no experiments have been conducted on the strongly stable boundary layer (SBL), because of the limitations in the commonly used facilities, i.e., wind tunnels and towing tanks. As discussed by Odell and Kovasznay (1971) and Stillenger et al. (1983), wind tunnels cannot simultaneously produce strongly stable stratification and high winds, both needed for a well-developed boundary layer, and towing tanks permit only very short duration experiments.

Stillenger et al. (1983) described a continuous-flow water channel that can produce arbitrary velocity profiles in combination with stable density gradients (by salt addition). Although this facility cannot simulate all aspects of the atmospheric SBL (e.g., Coriolis and nonstationary effects), it

could be used to study a steady boundary layer over a range of stabilities. Perhaps such a facility could also be used to study the time response of the boundary layer to changes in the surface heat flux, and to gravity waves.

Laboratory tow tank experiments have substantially advanced our knowledge of stably stratified flows about hilly terrain. For example, the experiments of Riley et al. (1976) and Hunt and Snyder (1980) for axisymmetric hills showed that below a stability-dependent height, the flow was essentially horizontally layered, while above that height, fluid passed over the hill. Similar results were obtained for a long ridge notched by a gap (Baines, 1979; Weil et al., 1981), but the depth of the horizontally layered regime was less than for the round hill. Both sets of experiments were consistent with Drazin's (1961) theoretical predictions on the existence of the horizontally layered regime.

Currently, a controversy exists about the dependence of the flow field on the hill aspect ratio (across-wind width to hill height; Snyder et al., 1983). The key issue is the nature of the upstream influence (and blocking) for a very large aspect ratio hill within a strongly stable flow and whether flow-field results, untainted by end-wall wave reflections, can be obtained in a tank of finite length. A solution to this controversy may require new and clever experimental techniques, but should be pursued because it bears on the future of laboratory modeling of stratified flow over terrain.

b. Diffusion Experiments

Laboratory simulations of point-source diffusion in the PBL have been conducted to test theoretical predictions and to gain new fundamental understanding. In the following, we discuss such simulations for both buoyant and nonbuoyant tracers, with a view toward what has been done and what is needed.

Neutrally buoyant tracers. Diffusion of neutrally buoyant tracers has been studied much more extensively in neutral and convective cases than in stable, primarily because of the difficulty of simulating the latter.

Neutral boundary layer. Diffusion in neutral (NBL) or weakly stratified boundary layers has been well explored because of its ease of simulation, at least in the absence of Coriolis effects. Although one might question the applicability of these simulations in view of the rarity of neutral conditions

in the atmosphere, we believe that they are useful as a limiting case from which diffusion in convective or stable conditions departs.

Wind-tunnel experiments provided some of the earliest convincing evidence (e.g., Cermak, 1963; Poreh and Hsu, 1971; Chaudry and Meroney, 1973) that vertical diffusion from a surface source can be described quite well by similarity theory (Monin, 1959). As a result of these and other experiments, in both the laboratory and field, we have a fairly good understanding of surface-source diffusion.

Comparable understanding does not exist for diffusion from elevated sources. Wind-tunnel tests show that the Gaussian-plume model is a good empirical description of diffusion from such sources. None of the conventional theories--statistical, similarity, and gradient-transfer--applies to the elevated source in the NBL, at least in the near-source region (Robins and Fackrell, 1979). An adequate theoretical description requires an improved understanding of the basic scalar transport mechanism in an NBL and, in particular, the transfer by the large eddies. Wind-tunnel measurements (Fackrell and Robins, 1982) should continue to contribute toward understanding of concentration fluxes, but further measurements are needed to delineate the role of the large eddies. Additionally, measurements of the probability distributions of the vertical and lateral velocity fluctuations (including their vertical profile) would be useful to advance and test Lagrangian statistical models of elevated-source diffusion.

The Fackrell-Robins measurements have also provided benchmark understanding of concentration fluctuations in turbulent plumes. They show the important difference between the intensity (rms/mean) of fluctuations for elevated and surface sources in wind tunnels. Along the tunnel floor in the near-source region, the intensity for the elevated release exceeds unity and is substantially higher than that for the surface release. The difference is due to the presence of smaller eddies near the surface. However, large lateral eddies can cause the concentration fluctuation intensity in the atmosphere to be high even near the surface, so that these results are not completely representative of atmospheric behavior. These measurements already have been used in the development and testing of theoretical models (Lewellen and Sykes, 1983), but more experimental investigation, a closer interplay with theoretical modeling, and better understanding of the large-eddy structure of the PBL are required to make progress on this important topic.
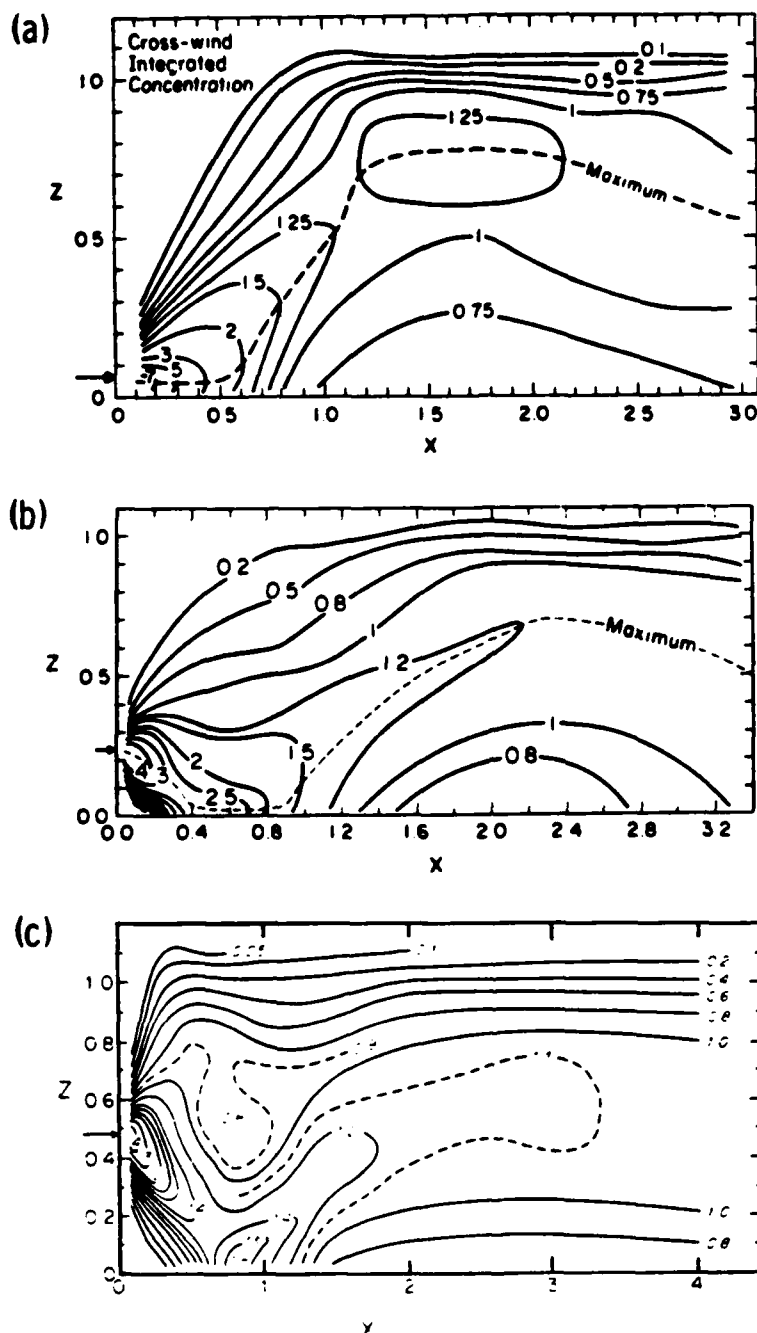
Figure 3. Laboratory convection tank results showing nondimensional crosswind integrated concentration (CWI) as a function of dimensionless height, Z, and downwind distance, X, for sources at three release heights in a convective boundary layer (CBL). The CWI is nondimensionalized by Q/uz_i, where Q is the source strength, z_i is the CBL height, and u is the mean wind speed. $Z = z/z_i$ and $X = w_*x/(uz_i)$, where z is the height above ground, and w_* is the convective velocity scale. Horizontal arrows denote the release height z_s: a) $z_s/z_i = 0.067$ from Willis and Deardorff (1976), b) $z_s/z_i = 0.24$, from Willis and Deardorff (1978), and c) $z_s/z_i = 0.49$, from Willis and Deardorff (1981).

Convective boundary layer. One of the most important recent advances in our understanding of PBL diffusion resulted from the laboratory convection tank simulations by Willis and Deardorff (1976, 1978, 1981), who simulated diffusion from release heights of $0.07z_i$, $0.24z_i$, and $0.49z_i$. They showed that for the lowest source height the plume centerline ascended after a short travel distance, whereas the centerlines from the more elevated releases descended until they intercepted the ground (see Figure 3). The diffusion patterns were quite different from those predicted by a conventional Gaussian-plume model. The descent of the elevated plumes is due to the organized, long-lived thermal motion in the mixed layer and to the larger area occupied by downdrafts than updrafts; the ascent of the near-surface plume results from the "sweep-out" of material near the surface by updrafts before the material aloft recirculates down. These unique simulations were recently verified in a field experiment reported by Moninger et al. (1983).

Although vertical dispersion in the CBL is well simulated by the Willis and Deardorff experiments, the cross-wind spread of the laboratory plumes appears to be about 25% smaller than that observed in the field, based on Nieuwstadt's (1980) analysis. This is probably due to the small aspect ratio of the convection tank, which limits the size and magnitude of the horizontal eddies.

Deardorff and Willis also have conducted simulations of two other important problems: fumigating of an elevated plume into an entraining mixed layer and surface concentration fluctuations due to an elevated release.

These simulations have been important not only in advancing fundamental understanding of CBL diffusion, but also in providing the stimulus, guidance, and data for the development of improved theoretical models. The simulations could be extended in a number of ways, some of which overlap with our earlier discussion of CBL structure.

One extension is the installation of a tank of much greater aspect ratio to see if the cross-wind dispersion more closely matches the field observations. One could also see if the Lagrangian time scale for the lateral fluctuations increases over previously determined (laboratory) values ($\sim 0.6z_i/w_*$) to produce a linear dependence of σ_y on travel time over a greater range of time (Deardorff, 1982).

A second extension is the simulation of diffusion in the near-neutral limit, say $-z_i/L < 2$. In particular, one wishes to know how diffusion patterns in the CBL approach those in the NBL as $-z_i/L$ approaches zero. Such simulations would require an experimental facility that simulates both surface friction and convection effects.

The third extension is the simulation of dispersion in very light winds when axial diffusion becomes important; i.e., as the ratio of mean wind speed, U, to the convective velocity scale, w_*, becomes small, say $U/w_* < 1.5$. Experiments should also be conducted in the limit of zero mean wind. The second and third extensions would then give us a picture of passive tracer diffusion in the CBL over the full range of stabilities.

A fourth extension is the measurement of the mean concentration field for sources in the upper half of the CBL. Field observations (Caughey et al., 1983) show that above $z/z_i \sim 0.75$ the probability density function (pdf) of vertical velocity is symmetric, the probability of downdrafts and updrafts being the same. Thus, one would not expect the plume centerline to descend as it did for releases at $0.24 z_i$ and $0.49 z_i$. However, these pdf observations differ from those computed numerically by Lamb (1982). Lamb finds the pdf to be positively skewed at heights up to and exceeding $0.75 z_i$. In addition, his numerical simulations of a release at $0.75 z_i$ show centerline descent.

Finally, we encourage the continuation of concentration fluctuation measurements for sources at a variety of release heights.

Stable boundary layer. Aside from simulations in the weakly stable surface layer, laboratory experiments on diffusion in the SBL do not exist because of the difficulties of producing a strongly stable boundary layer. However, given the prospects of the Stillenger et al. (1983) facility, such experiments should indeed be pursued.

In particular, diffusion experiments in a stationary, turbulent SBL could help determine the applicability of a theory by Pearson et al. (1983). The theory predicts that at long travel times, the vertical plume width (σ_z) can be constant and of order σ_w/N, where σ_w is the rms vertical turbulence velocity and N is the Brunt-Vaisala frequency. This result differs from statistical theory (Taylor, 1921), which predicts that σ_z varies as $t^{1/2}$ in the large-time limit.

Pearson et al. found that their theory agrees with diffusion measurements in stably stratified grid turbulence (see also Britter et al., 1983), but these results have been questioned because of the time decay of the turbulence in the experiments. They also cite field measurements of a power station plume exhibiting a constant vertical thickness with distance; however, this plume was 150 m above ground and may have been in a nonturbulent region above the SBL. Laboratory measurements in an SBL with nondecaying turbulence could assess the validity of this new theory.

Another area for new laboratory experiments is plume diffusion on the upstream side of hills in stably stratified flow. Experiments for axisymmetric hills in a uniformly stratified environment (Snyder and Hunt, 1983) show that the maximum concentration on the hill is approximately equal to the plume centerline concentration in the hill's absence, in agreement with theory (Hunt et al., 1979). These experiments need to be extended to hills of aspect ratio much greater than 1 and to other density distributions, e.g., a well-mixed layer capped by an inversion.

Obstacle wakes. Laboratory experiments have been our principal source of information on flow structure and diffusion in wakes. A major area has been diffusion in building wakes, where the issues range from the minimum stack height for avoiding plume downwash to the variation of plume widths with stack height, building geometry, and distance. Much of this work has been summarized by Hosker (1982).

Generic studies have been conducted for isolated buildings, thus enabling much of this work to be transferred to a variety of situations without the need for case-by-case simulations. However, for unusual geometries, especially clusters of buildings, results are difficult to generalize and probably would require separate laboratory simulation for each new situation. Thus, experimental facilities (such as those used by Cermak and colleagues at Colorado State University) will continue to be needed for these problems for the foreseeable future.

Experimental investigations of dispersion in hill wakes have been performed by Castro and Snyder (1982), with an emphasis on the effect of hill aspect ratio, stack height, and stack position relative to the "cavity," the recirculating, highly turbulent region immediately aft of a hill. As might be expected, Castro and Snyder found that the maximum and minimum concentrations

occurred for stacks downwind of ridges and round hills, respectively. The maximum concentration downwind of the ridge was as much as a factor of 10 greater than in flat terrain. The cavity for the ridge extended downwind to about ten ridge heights, and surface concentrations were enhanced over an extensive downwind distance.

While these studies have been quite informative, practically all have been conducted in neutral boundary layer flows. Experiments in stably stratified flows, where the potential exists for even higher concentrations, are needed, especially for the hill-wake problem. Concentrations would be expected to become most enhanced for moderate-to-large hill Froude numbers ($F > 1$) when an extensive wake occurs.

Buoyant plumes. Laboratory experiments have shown the behavior of buoyant plumes under a variety of ambient stratifications. Here we will discuss only the experiments on positively buoyant plumes. Meroney (1982) discusses wind-tunnel simulations of negatively buoyant plumes, and a survey of important problems, field observations, and modeling of dense gas dispersion can be found in a collection of papers edited by Britter and Griffiths (1982).

Laboratory experiments of plume rise and dispersion downwind of a tall stack have been conducted in neutrally stratified towing tanks (e.g., Hoult and Weil, 1972) simulating a laminar crosswind. Results of the mean plume trajectory (rise vs distance) agree with both field observations and a simple entrainment model for plume rise (Briggs, 1982; Weil, 1982). However, as shown by Fay et al. (1970), the pdfs of the entrainment parameter and individual rise realizations are much narrower in the laboratory than in the field, undoubtedly due to the absence of turbulence in the laboratory simulations. As shown by Hoult et al. (1977), a reasonably good match of the field and laboratory pdfs can be obtained, at least for short stacks, by simulating the atmospheric boundary layer.

The mean trajectory and final rise of a buoyant plume in a stable, uniformly stratified environment has also been successfully simulated in both wind tunnels (Hewett et al., 1971) and towing tanks (Lin et al., 1974). Since these simulations were done in a laminar crosswind, they do not display as broad a scatter in rise realizations as do field data. The above two problems--final rise in a stable environment and the mean plume trajectory near the source--are now well-understood.

Another important problem that has been simulated in a towing tank is the penetration of thin elevated inversions by buoyant plumes (Manins, 1979). The results show that penetration commences when the maximum plume density excess at the inversion base exceeds the inversion density jump. Although this result might have been expected, a previously used, simple theoretical model (Briggs, 1975) predicted penetration based on buoyancy depletion of the entire plume cross section at the inversion base; this approach significantly overestimated the degree of penetration.

Extensions of these experiments to a variety of inversion strengths and thicknesses can bear directly on the problem of predicting stack-plume dispersion under an inversion. In addition, experiments need to be conducted in the presence of convection below the inversion, i.e., in a CBL, since the convection will surely affect the degree of penetration and the dispersion.

Probably the most important and perplexing plume-rise problem remaining to be solved is the effect of ambient turbulence at large distances, where the possibility exists of a "final rise" caused by such turbulence (in the CBL or NBL). Very little field data exists on this subject; thus, theoretical models are based on rather simple and speculative assumptions, with little testing. We believe that this is a problem area where laboratory experiments can lead to great gains.

Willis and Deardorff (1983) recently completed some preliminary laboratory work on plume rise within the CBL. Their results showed the looping character of full-scale plumes and much broader ensemble-averaged plume outlines than found without ambient convection. They also suggested that the conventional two-part Gaussian model--plume rise plus ambient dispersion--is inappropriate; i.e., source-buoyancy and ambient-convection effects need to be considered simultaneously.

These experiments should be extended in a number of ways. First, more emphasis is needed on plumes with sufficiently low buoyancy flux that the mean rise is terminated well within the CBL, i.e., rise limited by ambient convection and not by the stable layer capping the mixed layer. Such experiments will show when and where the buoyant plume behaves more or less passively. Second, experiments are required on the partial penetration of the capping inversion by buoyant plumes and the dispersion of material trapped within the CBL. Third, experiments are needed over a full range of stability

conditions--from very light winds (U/w_* < 1.5) to near-neutral stability
($-z_i/L$ < 2). Experiments simulating final rise in the limit of a NBL could be
conducted in a wind tunnel. Fourth, measurements of surface concentration
fluctuations should be continued. Deardorff and Willis (1983) have already
made some such measurements and find that the maximum intensity of
fluctuations is greater for a buoyant than a neutrally buoyant plume from an
otherwise identical stack.

2.4 Atmospheric Experiments

Laboratory experiments are an attractive means of studying PBL processes,
in part because experiments in the PBL are so difficult and expensive. Some
of the obstacles to "direct" (atmospheric) experiments are:

1. The averaging times (or lengths, for aircraft measurements) required
   to minimize inherent uncertainty (see Eq. 1.1) are often longer than
   allowed by the diurnal cycle (or by local homogeneity). Some (e.g.,
   Wyngaard, 1983) have suggested, in fact, that area averaging might
   be required for particularly troublesome statistics, such as
   stress. As a result, many runs are typically required to reduce
   scatter to acceptable levels.

2. Mesoscale eddies, bad weather, and other unpredictable phenomena
   often make conditions nonstationary during PBL measurements and add
   noise to the desired signals. Laboratory experiments, by contrast,
   can often be designed to be precisely stationary.

3. The much larger range of spatial scales in the PBL makes it
   inherently more difficult to measure than laboratory flows. For
   example, the vastly larger Reynolds number in the PBL makes its fine
   structure much more intermittent and consequently more elusive.

4. While some have predicted that remote sensing would revolutionize
   boundary-layer meteorology, to date it has been useful primarily in
   flow visualization and in measurement of gross parameters such as
   PBL depth. Traditional (in-situ) sensors remain the standards for
   detailed, quantitative measurement of PBL structure. Not only are
   these sensors typically more expensive than their laboratory
   counterparts (e.g., sonic anemometers cost more than hot-wire
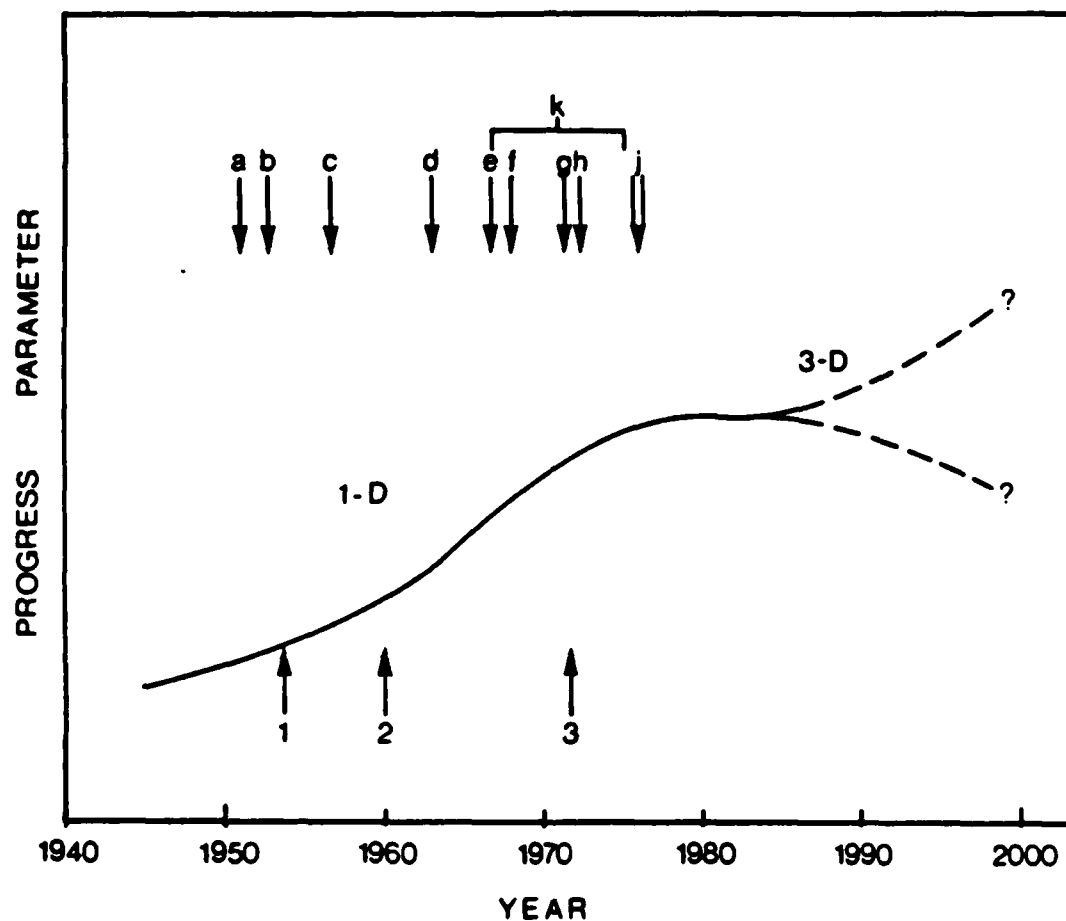
Figure 4.   Progress in boundary-layer research in the last three decades.
             Theoretical/numerical milestones: (1) Monin-Obukhov (1954); (2)
             Monin-Kazanski (1960, 1961); (3) Deardorff (1972). Experimental
             milestones: (a,b) Anegada, Scilly Isles observations (U.K.); (c)
             Great Plains observations (U.S.); (d) Kerang, Hay observations
             (Australia); (e) Wangara observations (Australia); (f) Kansas
             observations (U.S.); (g) Minnesota observations (U.S., U.K.); (h)
             Koorin observations (Australia); (j) AMTEX, GATE (international);
             (k) impact of remote sensing of boundary layer. From André et al.
             (1982).

anemometers), but their use in the PBL also requires expensive platforms (tall towers, aircraft, or tethered balloons).

5. It can take several years to accumulate the experience, funds, and equipment needed to carry out a successful PBL measurement program. For example, the benchmark 1968 Kansas expedition (Haugen et al., 1971) of the Air Force Cambridge Research Laboratories was actually the last of three experiments, the first two serving only as tests of experiment design and instrument performance. The 1968 version covered most of the summer and involved about 15 personnel in the field and perhaps ten full-time over the next three years in data processing and analysis. Nonetheless, history will undoubtedly record these experiments as good value, even though the data extend only to 32 m height, perhaps 2% of the daytime PBL depth.

In spite of the inherent difficulties with direct measurements, they have given us remarkable insight into the structure of the lower portions of the PBL. Experimenters have wisely restricted their studies to idealized cases (quasi-stationary, locally homogeneous, flat terrain, good weather) and have carefully detailed the statistical behavior of the surface layer.

The WMO Working Group on Atmospheric Boundary Layer Problems has charted (André et al., 1982) this progress schematically in Figure 4. The WMO group advanced two reasons for the steady progress evident from the early 1950s to the mid-1970s. First, several major field programs (listed in Figure 4) provided an extensive data base. Second, concurrent theoretical work was closely coupled to this experimental activity and provided the framework for interpreting the data. This interaction between theory and experiment led to effective parameterizations for many important aspects of PBL structure.

The WMO group suggested, however, that progress in this "one-dimensional" era was diminishing, as indicated by the plateau in Figure 4. While they felt that progress in one-dimensional problems would continue, they saw the future challenges and opportunities to lie elsewhere--especially in the three-dimensional, mesoscale PBL field. However, they cautioned that this broadening of scope would severely strain the capabilities of experimenters to generate data bases of sufficient generality. To maintain progress, the WMO group encouraged

1.   development of more advanced instruments and experimental
     techniques;

2.   continued close coupling of theory and experiment; and

3.   the integration of numerical modeling into the scientific program
     contributing to the data base.

The LES Working Group notes, two years later, activity consistent with
these recommendations. For example, the proceedings of a recent AMS short
course, "Instruments and Techniques for Probing the Atmospheric Boundary
Layer," (Lenschow, 1984) have a strong emphasis on new techniques.
Theoretical work in environmental fluid mechanics continues, closely coupled
with experiment (see, for example, Nieuwstadt and Van Dop, 1982) in accord
with the second recommendation. With regard to the third point, our group
notes increased use of LES techniques in PBL research (as discussed further in
Chapter Five).

2.5 PBL Modeling

Our previous sections make it clear that much has been learned over the
past decade about the PBL. Some of this new knowledge came from modeling
studies--but, as is usually the case in turbulence research, most came from
observations, both in the laboratory and in the atmosphere.   Detailed
analyses of data from the Minnesota, Wangara, AMTEX, Koorin, and GATE
atmospheric experiments have been most valuable; they have, for the first
time, given researchers detailed insight into the structure of the entire
PBL. Until these experiments, researchers had to content themselves primarily
with data from the "tower layer," the first 100 meters above the surface.

These atmospheric data bases also contain inputs from a new generation of
sensors--acoustic sounders, for example--which in the early 1970s dramatically
revealed the shallow nature of the nocturnal PBL and the abrupt morning
transition to a rapidly deepening convective PBL. These new experimental
thrusts gave us for the first time a global view of the PBL, revealing through
flow visualization the striking differences between its daytime and nighttime
states.

On the modeling side, there were two developments of major importance.
The first was Deardorff's series of large-eddy simulations--the first computer

calculations of the details of convective PBL structure. Although they were
very expensive his simulation of the 24 hours of day 33 in the Wangara
experiment (Deardorff, 1974) took 360 hours on the NCAR CDC 7600 , they gave
an unprecedented wealth of information. Deardorff soon established from these
simulations the turbulent velocity and temperature scales for a convective
PBL--scales which are in standard use today--and effectively put an end to the
controversy about what determines the height of an unstable PBL.

While Deardorff was doing this pioneering work, second-order modeling was
also being applied to PBL flows for the first time. This approach was not new
(the equations are discussed in Reynolds' classic paper of 1895), but large-
scale computers now made it feasible computationally. The rash of activity
which ensued carried through the 1970s. Second-order modeling was soon being
applied to a host of PBL problems, ranging from studies of structure and
dynamics in unstable, neutral, and stable conditions to PBL parameterization
and turbulent diffusion studies.

Virtually all of this early work with second-order models involved the
wholesale use of closures developed a few years earlier for shear flows. A
generation or more of carefully made laboratory measurements had given a rich
data base, and the early experience with second-order models tested against
this data base was quite encouraging. It was relatively simple to adapt these
shear-flow models to geophysical flows by adding the necessary conservation
equations for buoyancy variables and adding the explicit buoyancy terms in the
velocity field equations. The closure expressions were not usually modified
to include buoyancy effects.

This combination of experimental and numerical modeling activity over the
past decade had one other important effect--it focused attention on the
inherent uncertainty issue. As a result, both modelers and experimentalists
are now much more aware of the significance of scatter in PBL measurements,
and much more sensitive in their interpretations of the discrepancies between
model predictions and experimental data. They know that models generally
predict ensemble-average properties, while experiments usually yield time
averages, and they understand the complication this brings to model
verification. In fact, as we mentioned earlier, we now recognize a need, in
some diffusion applications, for models which predict the inherent uncertainty
as well as the mean.

a. Ensemble-average Models

Any numerical solution for PBL fields necessarily involves averaged equations, since the computer requirements are otherwise impossible. If the basic governing equations (i.e., the equations for momentum, temperature, scalar contaminant) are averaged over an infinite ensemble of realizations, one obtains equations for the ensemble mean fields. These equations have the well-known "closure problem" that prevents their direct solution; it stems from the nonlinearity of the conservation equations--which, upon averaging in a random field, leads to unknown ("Reynolds flux") terms involving the correlations of the random field components.

The ensemble-averaged equations are the traditional ones in boundary-layer meteorology; they represent the essence of what we usually want to know. The averaging process removes a tremendous amount of complicated, burdensome detail. The closure problem brought on by ensemble averaging is currently dealt with in two ways: through eddy-diffusion parameterizations (first-order closure) or through higher-order modeling.

The traditional closure is the first-order type, which assumes the Reynolds fluxes are proportional to mean-field gradients, just as they behave in molecular diffusion. The key difference, of course, is that molecular diffusivity is a property of the fluid, while the eddy diffusivity (K) is a property of the flow. This leads to the principal difficulty with this closure: specifying the eddy diffusivity.

One approach is to specify K values at the outset. This is crude and unlikely to be successful because K, a property of the flow, is not known before the flow is known in some detail.

A second approach is to specify the functional dependence of K on other flow variables (e.g., to specify K profile shapes). This is better, but unfortunately the functional dependence of K on PBL parameters is still a research issue. Furthermore, these dependencies can be very complicated. Lamb and Durran (1978), for example, found that for continuous point source diffusion in the convective PBL, K depends on z, w_*, PBL depth z_i (all of which would be expected), but also on the source height.

A third alternative is to specify what might be called K dynamics, i.e., to carry within the model a routine which calculates the K field given the global conditions, using some dynamical framework. One way to attempt this is

through second-order closure, whereby one carries a set of equations for the Reynolds fluxes. This set is based on the exact second-moment conservation equations, but has its own closure approximations. This underlying closure problem in turbulence affects moment equations of all orders and has to date prevented any completely rational solution to the turbulence problem.

The second-moment equations explicitly contain a good deal of the physics expressed by K. However, the unknown terms which must be parameterized in these equations also contain much of the physics. This illustrates at once the lure of second-order closure and its intrinsic difficulty.

Since second-order models use the ensemble-averaged field equations, they attempt to predict directly the statistics of turbulence without dealing with its instantaneous, random details. They are much faster computationally than "brute force" techniques such as large-eddy simulation, but their closure problem is also much more difficult; approximations must be made for pressure covariances, molecular destruction terms, and third-moment flux divergences. The last ten years of PBL research have taught us that the first two of these are very important in the second-moment equations, and the success or failure of model predictions can hinge on the accuracy of their parameterizations. These parameterizations, however, must express the effects of the entire spectral range of turbulence, and we know that the energy-containing eddies in any turbulent flow tend to be very sensitive to their environment. Thus, while one might be able to tailor second-order closure parameterizations to a particular type of flow, many researchers now feel that there is no reason to expect that the model will perform as well in another type of flow.

Large-eddy simulation, by contrast, needs parameterizations only for the turbulent motions too small to be resolved by the three-dimensional grid. This task is much less demanding, because these smallest eddies are thought to be more universal, i.e., less sensitive to the details of the flow in which they are imbedded; it is also less important, because the flow dynamics do not depend critically on the details of these unresolved eddies.

b. Large-eddy (volume-average) models

An alternative to ensemble averaging is volume averaging. If the basic conservation equations are averaged over space rather than over the ensemble, we remove the smallest-scale turbulence components, thereby making it possible

to solve these equations numerically on a computer. The averaged equations govern the large-scale components of the fields--that is, the means plus the largest-scale turbulent fluctuations. Since the computed fields are still random, even (statistically) one-dimensional problems require a full four-dimensional space-time grid. This is also the strength of the technique, because one calculates explicitly the largest-scale turbulent motions as well as the mean fields; thus, it is called "large-eddy simulation" (LES).

The only closure parameterizations required in LES are those representing the effects of the subgrid-scale eddies. If the spatial grid is fine enough (on the order of 100 m in the convective PBL) to resolve the energy-containing eddies, the subgrid-scale eddies will not carry appreciable turbulent flux, however, and their parameterizations are not critically important.

A simple example might help to illustrate the difference between ensemble-average and volume-average models. Consider a field experiment with an array of sensors spaced 50 m apart in a cubical lattice, perhaps measuring temperature fluctuations with a fast response time. Suppose we examine the readout from each of these sensors only after the data have been time-averaged for a period of one hour. This averaged data from the sensor lattice would then have a character very similar to the output from a three-dimensional ensemble-average model. The averaging removes the turbulent randomness, which is desirable when we do not wish to deal with enormous detail. If we are to explain temporal trends in these average statistics, however, we must infer (parameterize) the behavior of the turbulent fluctuations that we have smoothed. The parameterization must account for the total turbulent flux divergence.

Now consider another experiment using a hypothetical remote sensor that measures the average temperature within a volume 50 m on a side. If this remote sensor could rapidly scan many such volumes, it would reveal the thermal structure of turbulent eddies larger than 50 m. If we also had wind velocity information on this scale, we could compute the turbulent fluxes associated with eddies larger than 50 m. This experimental output is analogous to that given by a volume-average model (LES). In this case, in order to explain temporal changes in the volume-averaged variables we need only infer (parameterize) the effects of turbulent fluctuations whose scale is less than 50 m. As the volume sampled by our remote sensor increases, we

increasingly lose information on the details of the turbulence field, and the
distinctions between the LES and ensemble-average models blur.

This analogy illustrates the distinction between LES and ensemble-average
models. But what, one might ask, is the primary difference in terms of the
actual coding of two such models? The answer lies in the nature of the
parameterization schemes needed to represent the unresolved turbulent
fluxes. The ensemble-average model, needing to parameterize the total
turbulent flux, generally utilizes an integral length scale that represents
the scale of the large, energy-carrying eddies. Only the subgrid portion of
the turbulent flux need be parameterized in the volume-averaged model; thus,
its length scale prescription can be directly related to grid spacing. In
practical terms, this means it should be possible to design a code in which
one can switch from an LES to an ensemble-average model simply by altering the
length scale prescription.

CHAPTER THREE
APPROACHES TO PBL MODELING

In this chapter we discuss in more detail the basic PBL modeling techniques in order to gain a broad perspective of "where we have been" and "where we are," and thereby to indicate areas ripe for advancement with LES.

3.1 Integral Models

In some applications one does not need detailed information about the PBL or about diffusion within it, but instead needs only gross properties. For example, one might want to predict the evolution of PBL depth or surface fluxes or the plume centerline concentration downwind of a continuous point source of pollution. What are known in engineering as integral models are appropriate *for such applications.*

Boundary-layer meteorologists know integral models by the terms mixed-layer models, slab models, or PBL-depth models. As in engineering, they are derived by integrating a governing equation (mean momentum, temperature, scalar concentration, turbulent kinetic energy. . .) between the surface and the PBL top. One must specify certain profile shapes in order to do this integration, and these are usually obtained from experiments. This general approach has been widely used in boundary-layer meteorology in the past decade, yielding daytime entrainment and inversion-rise models (Mahrt and Lenschow, 1976; Driedonks, 1982); nocturnal PBL depth models (Nieuwstadt and Tennekes, 1981; Stull, 1983); geostrophic drag law models (Wyngaard, 1983); a nocturnal jet model (Zeman, 1979); and a parameterization scheme for scalar transport through the convective PBL (Wyngaard, 1984).

Gaussian-plume models for pollutant dispersion are integral models as well; the mean concentration profile is specified (Gaussian) and the scalar conservation equation integrated over space to provide constraints on the centerline concentration. Briggs' (1975) plume-rise equations are another example of the successful use of the integral approach.

As normally constituted, integral models predict only mean properties and, by their nature, provide no new information on distributions within the PBL. That information comes from what boundary-layer meteorologists call "high-resolution" models, which we describe next.

3.2 Ensemble-average High-resolution Models: K, Second-order Closures

We saw earlier that ensemble averaging of the governing PBL field equations creates unknown second-moment terms (Reynolds fluxes). By analogy with molecular diffusion, first-order (K) closures replace these unknown turbulent fluxes with the product of an eddy coefficient and the appropriate mean gradient. The closure problem thus is shifted to one of prescribing an eddy coefficient.

Early PBL models set K equal to a constant, or some simple function of height; this permitted analytic solutions to PBL structure, of which the Ekman spiral is a familiar example. Prandtl mixing length methods set K equal to the product of a velocity scale and a length scale. The focus then switches to specification of the length scale ℓ (the velocity scale generally being determined from the mean flow speed), and a common approach has $\ell \propto z$ near the surface and ℓ constant aloft (Blackadar, 1962). A more modern approach directly specifies the shape of the vertical K profile throughout the PBL, with the magnitude of K being controlled by similarity expressions for K in the surface layer (O'Brien, 1970). The latter technique has been used extensively by Pielke and his colleagues (Segal et al., 1982; McNider and Pielke, 1981; Pielke, 1974) in dynamic PBL modeling on the mesoscale.

Other K-closure variations compute the eddy coefficients by using the local mean wind shear and buoyancy through a local Richardson number and/or a local mean strain rate. This approach allows the character of the flow, as it evolves, to determine K.

On balance, however, K-closure has severe limitations when considered against the real complexities of atmospheric turbulence. Experience with geophysical flows has shown that only rarely outside the surface layer are turbulent fluxes and mean gradients so simply related. A recent LES study by Wyngaard and Brost (1984), for example, shows that K-closure is incorrect in principle for scalars diffusing through the convective PBL. The necessity of

providing a length-scale prescription can further restrict its utility. (See Corrsin, 1974, for further discussion of this topic.)

Indeed, it is the surprising degree of success of K-closure models, despite many apparently valid objections, which ultimately requires quiet contemplation. Perhaps much of the answer is to be found in the nature of the problems most frequently addressed in PBL modeling. Until recently the range of flows simulated by PBL models has been relatively narrow, compared to the wide variety of flows addressed in the laboratory. For example, in PBL applications there generally are no recirculation, wake, and separation phenomena, or multiple boundary layers (although buoyancy, phase-change, radiative transfer, and terrain-induced processes can add considerably to PBL complexity). Thus, often in PBL problems it is possible in a rough way to specify a single integral length scale proportional to PBL depth. Once the proportionality factors appearing in the eddy coefficient expression have been adjusted to transport roughly the correct amounts of momentum and heat for this simple class of PBL flows, then one generally has a model which will give useful answers for different wind speeds, shears, and stratifications, as long as the overall character of the flow being simulated is unaltered.

The failure of K-models to handle more complex flows, particularly those in the laboratory, coupled with the increasing availability and power of computers in the 1970's, provided impetus to the development of second-order closures. Major production terms that require no approximation appear in the second-moment equations, thus making it attractive to add these to the set of equations for the mean field. One is thus able to carry expressions describing the time history, turbulent transport, and nonlocal effects missing in K-closure. However, unknown terms (some rather obscure looking at first) also appear in these second-moment equations; these terms must be modeled to achieve a closed set of equations, and it is the fidelity of such parameterizations to the true turbulence dynamics that ultimately determines the accuracy and reliability of a second-order model.

As with K-models, second-order models must be calibrated against well-documented flows. This has been done extensively in the engineering community, where a variety of high quality, well-defined laboratory data sets can be used for judging model performance. The goal of some modelers has been to achieve a "universal" model which does not require new closure expressions

or new closure "constants" for each new flow type. While some workers feel
that turbulence itself is far too complex to permit universal modeling of this
type, some do feel that progress in this direction has been made. Lewellen
(1977) describes numerous flow simulations, both laboratory and geophysical,
that have been made with one second-order model.

Perhaps the most widely used second-order model in meteorological
applications is that developed by Mellor and Yamada (1974; hereafter, M-Y).
They present a hierarchy of different closure model formulations, differing in
the number of approximations made in the second-moment equations. The M-Y
hierarchy of models has been used by different investigators to simulate
laboratory shear flows, stabilization by flow curvature, the stability
dependence of turbulence within the atmospheric surface layer, free convective
growth of the PBL, the diurnal PBL behavior, pollutant dispersion, two- and
three-dimensional flow with orography, stratus-capped, foggy, and cumulus-
containing boundary layers, the behavior of the oceanic mixed layer, vertical
turbulent fluxes for a general circulation model, and operational forecasts of
microwave refractivity. In a recent review article (Mellor and Yamada, 1982)
the authors point out that this modeling success has been achieved, even
though the empirical constants appearing in the closure expressions are
derived from neutral laboratory flow data.

And yet, as might be expected of a model which has been in existence long
enough to have received such heavy use, the Mellor and Yamada formulation is
now known to have deficiencies in several of its closure assumptions. As we
mentioned earlier, second-order closure models require parameterization of
three types of terms: triple-moment, pressure-strain rate covariances, and
molecular destruction rates.

Most second-order models (including the M-Y) treat the triple-moment
terms as a downgradient diffusion process, since this has been found to work
well for laboratory shear flow simulations. In geophysical flows, however,
buoyancy forces often play a very strong role in turbulent transport, and
Wyngaard (1973, 1980) shows that in the convective surface layer downgradient
diffusion is a particularly poor approximation--with quantities such
as $\overline{ww}^2$ being transported up-gradient. The vertical flux of turbulent kinetic
energy, $\overline{wq}^2$, is everywhere positive in the convective PBL, whereas
downgradient-diffusion models predict negative $\overline{wq}^2$ near the surface and

positive values aloft. This has led Lumley et al. (1978) to state that
". . . a layer powered by a gradient-transport model cannot behave properly,
and in fact the rise of the inversion base is very poorly predicted, while the
vertical distribution of turbulent energy is wildly in error."

Most second-order closures for the pressure-strain rate covariance use
heuristic arguments drawn from examination of a Poisson equation for
fluctuating pressure, which in turn is derived from the Navier-Stokes
equations. This Poisson equation indicates that (in neutral shear flows) the
pressure-velocity correlations are governed by two contributions: turbulence-
turbulence interactions and turbulence-mean shear effects. The former term is
invariably modeled in a manner suggested by Rotta (1951), i.e., as a "tendency
towards isotropy" term. This term acts to redistribute energy components
towards an isotropic state without altering the total amount of turbulent
kinetic energy. However, Wyngaard (1980) found that this Rotta
parameterization does not properly represent the observed behavior in the
atmospheric surface layer.

There are several methods for parameterizing the turbulence-mean shear
contribution to the pressure-strain correlation. Perhaps the most widely used
form is that proposed by Launder et al. (1975), which also takes on the form
of a "tendency to isotropy"--but in this case it is the production tensor
(shear plus buoyancy) that is being redistributed towards a more isotropic
state. Mellor and Yamada use a form of this term that contributes only to the
off-diagonal elements of the stress tensor, and further modify it with a very
small coefficient that reduces its importance. However, most parameteri-
zations ignore buoyancy effects.

The final type of term requiring closure, the molecular destruction term,
is usually parameterized as

$$2\nu \left\langle \frac{\partial u_i}{\partial x_k} \frac{\partial u_j}{\partial x_k} \right\rangle = \frac{2}{3} q^3/\ell \; \delta_{ij} \tag{3.1}$$

in the case of the Reynolds stress equations. Here q^2 is twice the turbulent
kinetic energy, ν the kinematic viscosity, and ℓ is a length scale
characteristic of the energy-carrying eddies. However, Wyngaard (1980) shows
that this parameterization requires ad hoc adjustment to account for observed
PBL behavior over a range of stabilities.

The results from second-order models under convective conditions seem considerably better than one might expect, given the weaknesses in their closures. Figures 5-7, from Mellor and Yamada (1982), show some results of their second-order model simulation of the laboratory convection tank experiment of Willis and Deardorff (1974). The agreement with the measurements is good. This illustrates that the overall performance of a second-order model can be better than that of its various closure parameterizations, because these parameterized terms are not always vitally important. For example, near the surface, where the sign of $\overline{wq^2}$ is wrong when it is parameterized as downgradient diffusion, production and dissipation terms dominate, and transport plays a relatively minor role. Perhaps the biggest concern arises from the underestimation of the downward heat flux at the top of the convective layer in models using downgradient transport. Models which carry dynamic equations for the third-order transport terms have been developed and applied to a limited set of convective situations (Lumley et al., 1978; Sun and Ogura, 1980; André et al., 1976). The resulting distributions of third-order quantities are clearly improved in these models, whereas improvements in lower-order terms are more difficult to discern.

We must add, however, that second-order modelers of the PBL do not have access to "calibration" data sets of the scope and quality that laboratory flow modelers routinely expect. As we discussed in the previous section, much of this is due to the inherent uncertainty problem and to the great difficulty and expense of making PBL measurements. As a result, we actually know very little about the true behavior of the terms that are parameterized in second-order models, and not enough about the structure of the PBL to make definitive assessments of model predictions. Some researchers suspect, in fact, that some of our parameterizations are rather poor descriptors of nature, and that they (and perhaps some of our current models) survive only because of our ignorance of the real behavior.

The second-order modeling of Lumley and his colleagues is quite different from that generally practiced. Lumley has developed a more general approach to closure, one that emphasizes realizability constraints and tends to give more complicated closure expressions. This work is still in its relatively early stages and has yet to be exhaustively tested, but Lumley remains optimistic about its potential.
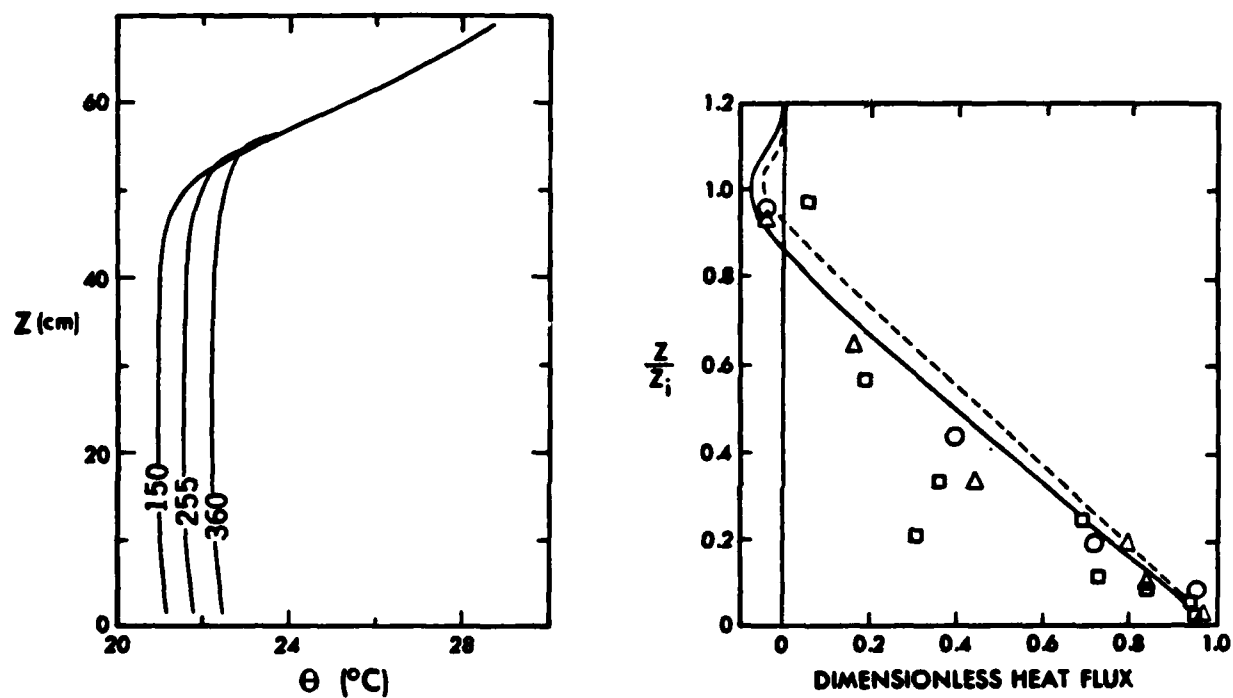
Figure 5.   Mean temperature and heat flux profiles from the laboratory
            experiments of Willis and Deardorff (1974).   Calculated profiles
            were nearly coincident with these curves.   Numbers on curves on
            left are seconds after runstart; curves on right are two different
            runs.   Open data points are atmospheric aircraft measurements in
            conditions thought to be similar to those of the laboratory
            experiment.   From Mellor and Yamada (1982).

Figure 6. Horizontal and vertical turbulent energy components (solid
symbols) by Willis and Deardorff (1974). Open data symbols are
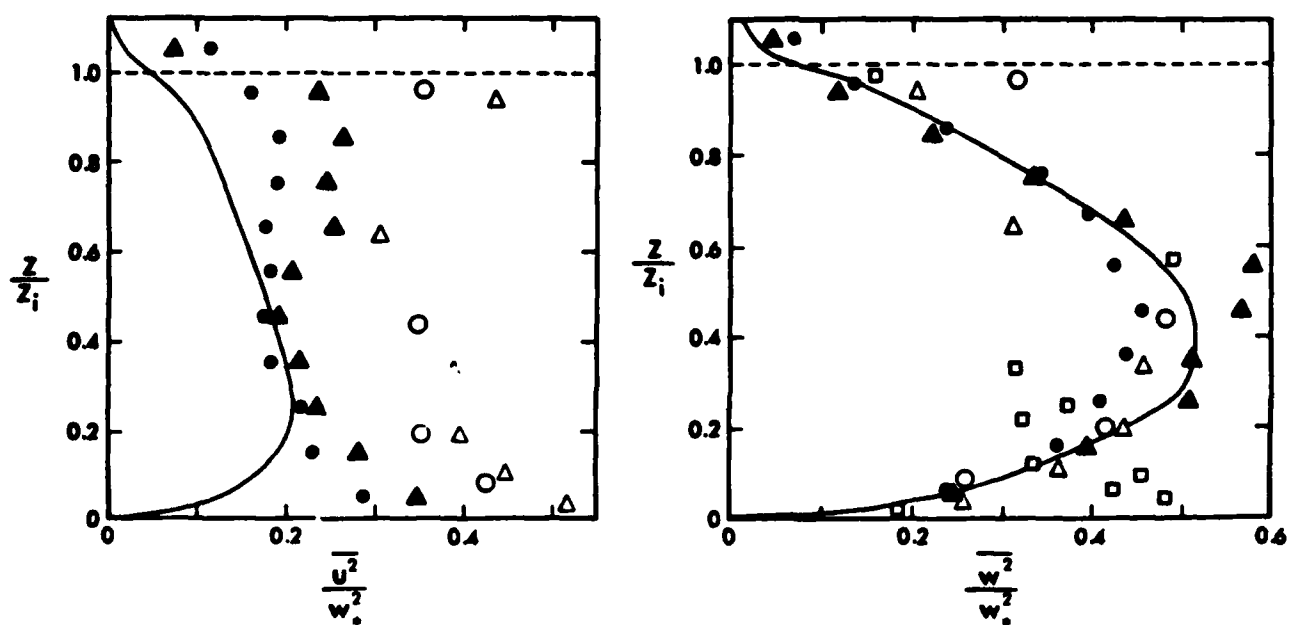aircraft measurements; solid lines are calculated. From Mellor
and Yamada (1982).
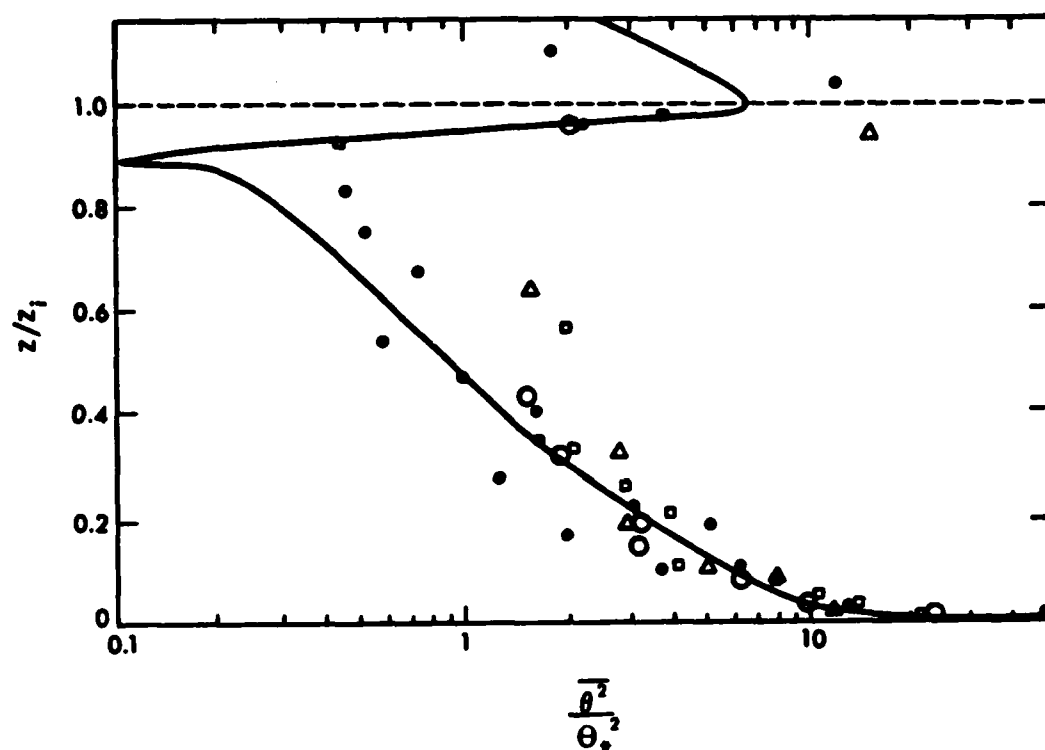
Figure 7.   Temperature variance (solid symbols) by Willis and Deardorff
             (1974). Open data symbols are aircraft measurements; solid lines
             are calculated. From Mellor and Yamada (1982).

Lumley has summarized his perspective of second-order modeling in a 1983
review paper. His section 3, "Performance of Existing Second Order Models,"
is particularly relevant here:

> Just as in the case of the first order models, such as mixing
> length or K-theory models, we are dealing with a calibrated
> surrogate for turbulence, albeit one that contains a little
> more of the physics. We would thus expect that the models
> would work satisfactorily in situations not too far removed
> geometrically, or in parameter values, from the benchmark
> situations used to calibrate the model. To the extent that
> more physics has been retained, we might expect the range of
> satisfactory performance to be greater. If the modeled terms
> behave correctly physically, there does not seem any reason
> not to hope for a very extensive range of satisfactory
> performance, supposing that the relevant physical mechanisms
> have been retained in the equations.

> In 1981-82 a competition was held (Kline et al., 1981) between
> various methods for calculating isothermal flows of
> engineering interest. Nearly all the methods in competition
> were either k-ε (. . . an eddy viscosity model in which the
> local value of the eddy viscosity is calculated), algebraic
> stress (. . . the Reynolds stress is given by an algebraic
> expression somewhat more complex than an eddy viscosity) or
> second order . . . . The conclusion of the judges was that
> the range of satisfactory performance of the models was rather
> narrow, and that we should probably expect to use for some
> time a variety of models optimized for particular geometrical
> situations and parameter ranges. The judges were split on the
> likelihood of ultimately improving this situation: the
> pragmatists felt that there was no objective evidence for
> putative universality, while the optimists (including the
> present author) felt that improvement of the physical behavior
> of the modeled terms held considerable hope. Most of the
> models have been constructed in a somewhat haphazard manner;
> as we shall see below, there are many restrictions which they
> should satisfy which are generally violated. Much of the
> modeling is not based on first principles, but is almost
> completely ad hoc. It seems there is enough room for
> improvement here to justify a certain optimism.

> Many of the initial successes of the models (in comparison to
> first order ones) have been in more complex flows, involving
> heat transfer, buoyancy and the like, because the relevant
> physical mechanisms are included. In addition, some of the
> successes have been in flows dominated by inertia or mean
> buoyancy, where the details of the turbulence model are
> irrelevant. Thus emboldened, the modelers have been
> overenthusiastic in promoting their models for other complex
> situations, often without considering at depth the difficult

> questions that arise. Consequently, there is some
> disillusionment with the models, a feeling that they embody
> too many ad hoc assumptions, and that they are unreliable as a
> result . . . . This reaction is probably justified, but it
> would be a shame if it resulted in a cessation of efforts to
> put a little more physics and mathematics into the models.

Lumley refers to the split between pragmatists and optimists on whether second-order models can achieve universality. In the engineering community there seems to have been a marked shift (numerically, at least) toward pragmatism. As research revealed the complex details of engineering flows, many researchers have concluded that there are as many kinds of turbulence as there are kinds of flow, and that it is unlikely that a single parameterization can apply to all situations. This pragmatic view has led to the concept of "zonal" modeling (Kline, 1981).

3.3 Volume-average High-resolution Models: Large-eddy Simulation

LES models are computationally demanding, requiring a three-dimensional grid in space plus stepping in time. In fact, they can easily require several orders of magnitude more computer time than integral models; K and second-order closure models lie in between. This spread is so striking that one would expect each to have its own optimum area of application, and this is broadly the case. Within some problem areas, however, there still is some healthy competition. For example, both integral and high-resolution PBL modules are used within current dynamical mesoscale models. As another example, second-order closure and LES compete in certain research applications, including some problems in turbulent diffusion.

Nonetheless, LES models are more faithful to the underlying physics than any other type of PBL model. Given that reality, our working group saw that one profitable use of LES is in testing and refining the simpler, faster models. For example, integral models require specification of mean profile shapes, which LES can provide. The Wyngaard-Brost (1984) LES results give scalar concentration profiles in the convective PBL as functions of the scalar fluxes at top and bottom and certain PBL turbulence parameters. Wyngaard (1984) used these results to develop a scalar transport module (an integral model) for the convective PBL. This could be extended to momentum profiles and to neutral and stable states. As another example, Lamb (1982) used

Deardorff's LES convective PBL velocity field to do continuous-point-source diffusion calculations. His results, (and those from the Willis-Deardorff tank experiments) are now being used to improve the Gaussian-plume models. It would be worthwhile to extend these LES studies to concentration fluctuations in order to quantify the inherent uncertainty in the predicted mean concentration fields.

We also see considerable potential for using LES models to develop improved second-order closure parameterizations. Since LES models can directly compute many of the details of the turbulence field that must be parameterized in second-order closure models, LES could provide a "numerical laboratory" for testing closure parameterizations, much in the same way that Deardorff's LES results have been used in developing turbulence scaling expressions. This could be particularly valuable, for example, if the LES resolution were sufficient to resolve directly most of the flux in the entrainment zone at the top of the convective PBL, since this is a region that has given ensemble-average models particular difficulty. In addition, the systematic study of turbulent pressure covariances through LES (some of which was attempted by Deardorff, 1974b) has the potential for improving their current parameterizations in second-order models. These very important terms are impossible to measure directly, and nearly impossible to parameterize rationally by other techniques. Rogallo's (1981) simulations of homogeneous turbulence provide an excellent example here. For a range of values of flow-parameters, such as Reynolds number and mean strain rate, he has tabulated the numerical values of terms in the Reynolds-stress equations, using his results from simulations on a 128 x 128 x 128 grid. These results provide an extensive data base for evaluating second-order-closure models. The improvement of second-order models based on LES results would also permit one to address more confidently some complex geophysical flows (e.g., flow in complex terrain; long-range dispersion) with ensemble-average models.

Selection of subgrid-scale parameterizations for LES models has often taken its guidance from techniques developed for ensemble-average closures; thus, improvements to second-order-closure schemes would hold strong promise for potential improvement in LES subgrid parameterizations. This, in turn, could permit the LES modeler to relax the grid-volume restrictions, if he had a more reliable subgrid-scale formulation. Generally the tradeoff of extra

model complexity for reduced resolution requirements is a good one, since doubling resolution in three dimensions can lead to a 2^4 increase in computing requirements (assuming that the time step is also linked to the grid spacing).

CHAPTER FOUR

LARGE-EDDY SIMULATION: AN ENGINEERING VIEW

The origins of what became large-eddy simulation (LES) lie in the early global weather prediction models. In developing these models, meteorologists quickly realized that the computer resources would permit only extremely coarse grids; in the early codes, the grid could hardly resolve the largest structures of the atmosphere. The unresolved scales require modeling or parameterizations, and considerable effort has been put into the development of these.

The first engineering application of LES was made by a meteorologist; Deardorff's (1970) pioneering paper provided many of the foundations of the subject and influenced much of the later work. Until now, application of LES has been limited to a small number of groups with access to the required resources. The increasing availability of large computers is allowing more groups to participate in LES.

The first work after Deardorff's was U. Schumann's thesis of 1973; following that, Schumann led a group at Karlsruhe that specialized in LES of convective heat transfer. W.C. Reynolds and J.H. Ferziger of Stanford began work in 1972 and have concentrated on developing the fundamental formulation of the subject, systematic extension to more complex flows, and application of the results of the investigations to turbulence parameterization. The NASA-Ames group, which began work in 1975, has specialized in state-of-the-art simulation of simple flows and on full turbulence simulation (see below). D.E. Leslie and his group in London began in 1976 to look at a number of issues, including the use of turbulence theories in developing subgrid-scale models. In the last few years, several French groups have begun to apply LES; these include those at Electricite de France, ONERA-Chatillon, Lyon, and Toulouse.

Full-turbulence simulation (FTS) simulates turbulent flows without any modeling. The number of accessible flows is much more limited with this approach, and the Reynolds numbers must necessarily be very small. The

pioneering work in this field was done by Orszag and his group at MIT in 1972. The method has since been applied by a number of other groups, principally those which also employ LES.

Due to the cost of the method, applications of LES to practical engineering flows have been almost entirely indirect until very recently. Recent advances in Very Large Scale Integration (VLSI) technology are producing dramatic reductions in the cost of a given computation; large computers should become available to a much wider group of users in the near future. This will make it possible for new groups to begin to use LES. The coming supercomputers will also open up new directions for research in this field.

4.1 Engineering Contributions of LES

As noted above, the cost of LES is very high. Consequently, runs have had to be selected with care. The choices have generally reflected the goals of the particular research group; to date, most simulations have been aimed at demonstrating potential and at exploring capabilities and limitations rather than at simulating flows of direct engineering interest.

This work has established that the conceptual basis of LES is sound. At very low Reynolds numbers, it is possible to do FTS where no modeling is needed. At somewhat higher, but still low, Reynolds numbers, LES captures most of the turbulence energy; the results are not sensitive to the subgrid-scale model used, and LES works well. Unfortunately, most applications require much higher Reynolds numbers, and here even the largest LES programs that can be run on present (or the anticipated next-generation) computers can capture only a small portion of the energy in some regions of the flow. In these cases, one will be asking much more of the subgrid-scale model, and a premium will be placed on the quality of that model.

In the remainder of this section, we will review some of the accomplishments to date with an eye towards results which are most likely to be of use in the future.

a. Method Demonstration

The first demonstration of the soundness of LES was Deardorff's 1970 paper. He showed that many features of turbulent channel flow could be simulated on a relatively coarse grid. The small-scale turbulence in the
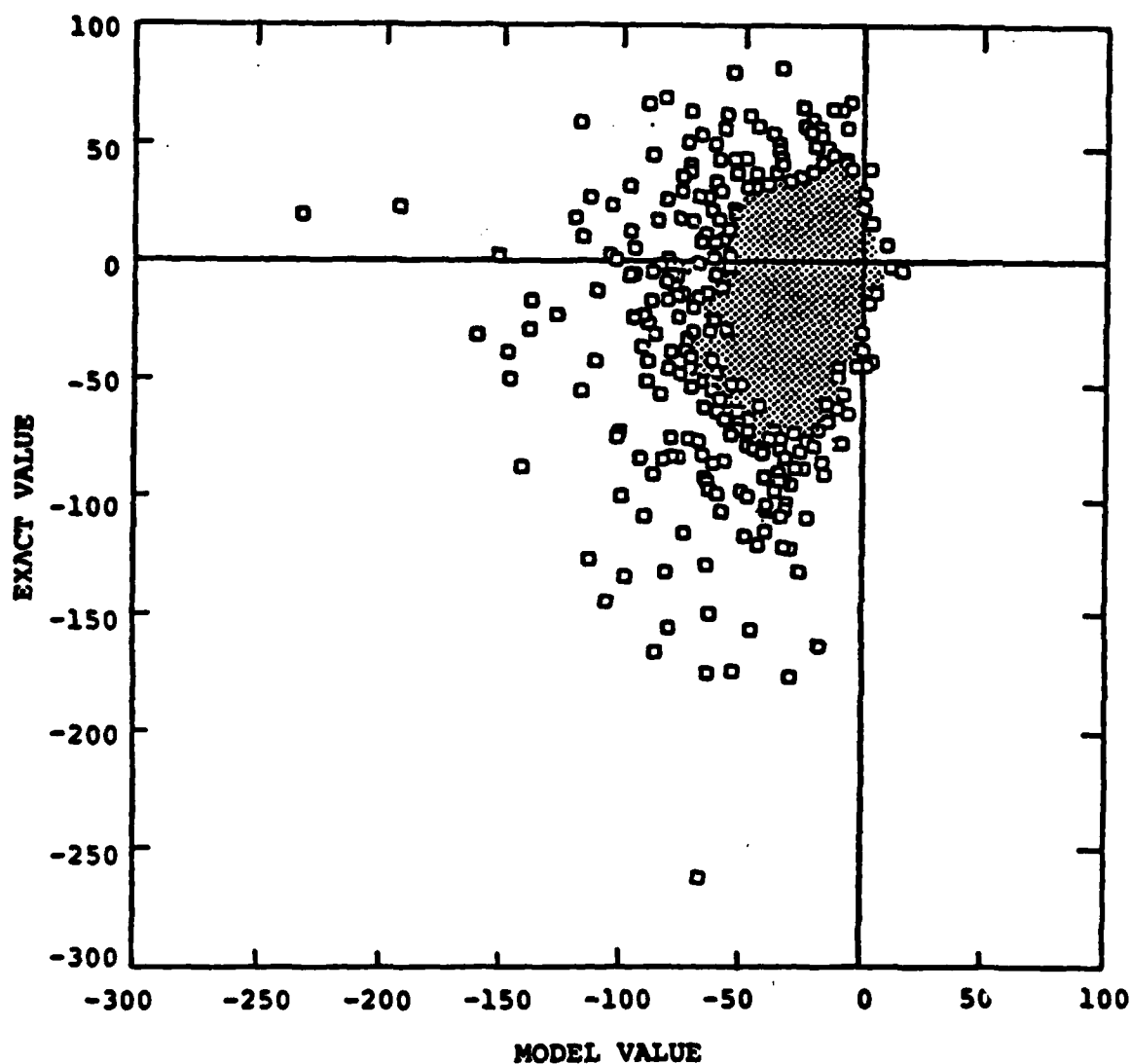
Figure 8. A test of Smagorinsky's model (parameterization) of the subgrid-scale Reynolds stresses. At each point in a test field, the exact value of the stress (obtained from a full simulation) is plotted against the value predicted by the model. An accurate model would produce a line at 45° line in this kind of plot. The correlation coefficient in this case is only about 10%, indicating that the model is poor on this detailed level. From McMillan et al. (1980).

Figure 9. A scatter plot similar to Figure 8 for the scale similarity model of Bardina et al. (1983). The correlation coefficient is now about 75%, a major improvement over the previous model. Source as in Figure 8.

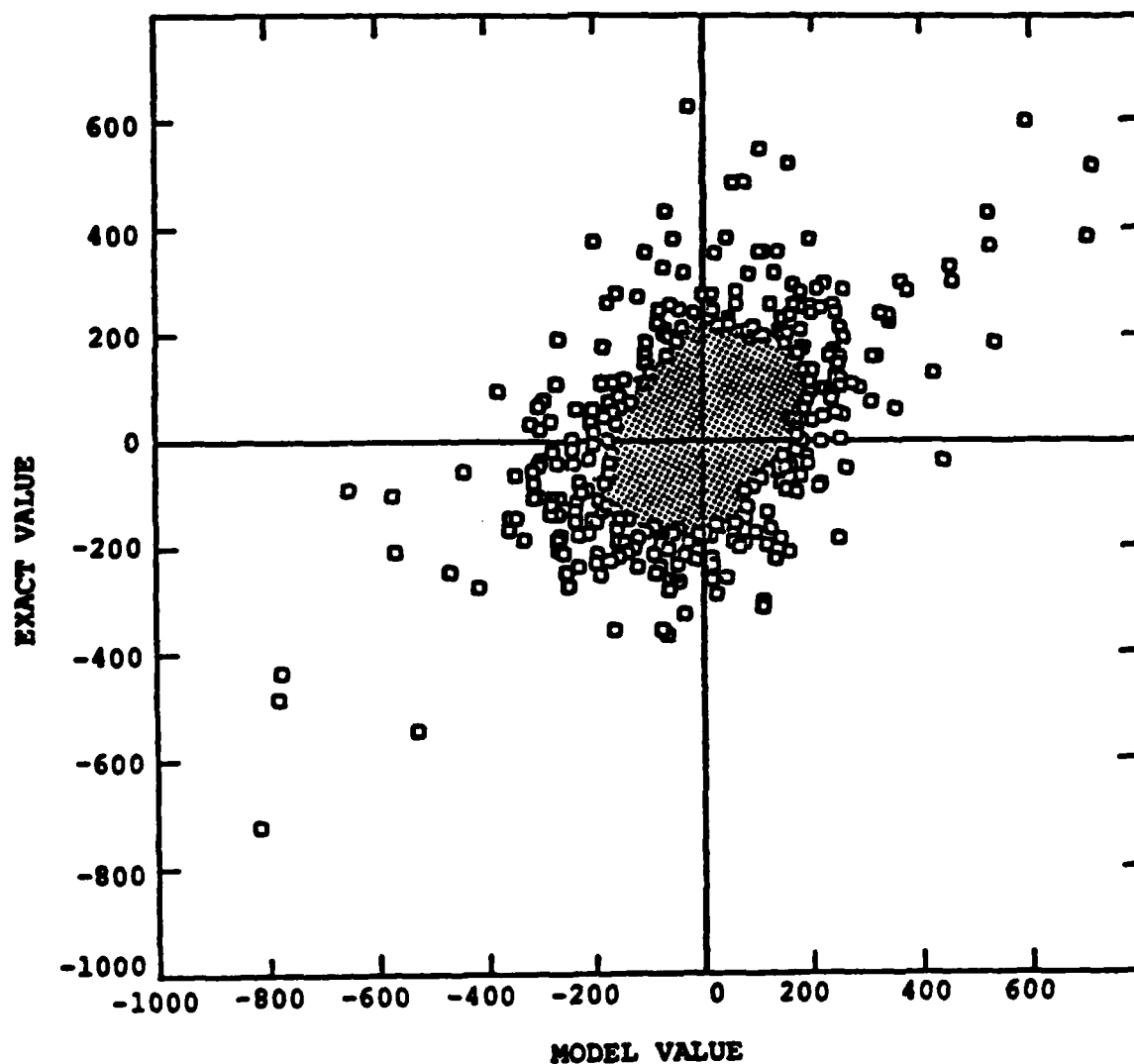center of the channel and the entire flow near the wall were treated by the subgrid-scale model.

The concept of filtering as a means of defining the large and small scales was introduced by Leonard (1973). Numerical approximations are completely separated from the filtering process in this approach, which the Stanford group has continued to use. Others prefer Deardorff and Schumann's method, which combines filtering and numerical approximation in a single step. The principal advantage of the two-step approach is that it simplifies thinking about what is to be computed and permits insights into the nature of subgrid-scale modeling that would be difficult to obtain otherwise.

The first flows considered by the Stanford group were the simplest, i.e., the various homogeneous turbulent flows. Kwak et al. (1975) and Shaanan et al. (1975) showed that LES could simulate isotropic turbulence with a model that is independent of grid size and the number of points used; this provided the faith that the subgrid-scale model was able to perform as intended.

Use of FTS to test subgrid-scale models was proposed by Clark et al. (1975) and was followed up by McMillan and Ferziger (1979, 1981). This work showed that Smagorinsky's model (which uses the local, resolvable-scale deformation rate and the grid size) represents the interaction between the large and small eddies well on the average, but poorly in detail; moreover, the model becomes worse when applied to sheared or strained flows. A scatter-plot test of this model for strained turbulence is shown in Figure 8. Its shortcomings led to a search for new models, which resulted in the scale-similarity approach proposed by Bardina et al. (1983) and the two-point turbulence closures of several French groups (Bertoglio et al., 1983 and Aupoix et al., 1983). These models are relatively new and untested, but hold promise for the future. A scatter-plot test of the scale-similarity model is given in Figure 9; it shows considerable improvement over the Smagorinsky model.

Next, it was decided to attack flows which are homogeneous in two directions--the time-developing free shear flows and the channel flows. The former were done by Mansour et al. (1978), Cain et al. (1981), and by Riley and Metcalfe (1981). The latter have been done by Schumann and members of his group, by Moin et al. (1978) and as described in a series of later papers, by Moin and Kim (e.g., 1981).

It was thought that free shear flows would be easier than wall-bounded ones because their physics is simpler. However, they are the most energetic turbulent flows, and their length scales grow rapidly; they eventually become larger than the computational region, at which time the simulation must be stopped. One would like to use a grid which grows with the flow, but unfortunately no one has yet found a method which accomplishes this without severe approximations. Some progress has been made; examples are Cain's method for infinite domains, which allows him to simulate the transition of a mixing layer almost to the point of full development, and the Riley-Metcalfe work on fully developed free shear flows.

In the area of wall-bounded flows, there has been considerable progress. Schumann and his co-workers, Grotzbach and Kleiser, have, in a long series of papers, extended Deardorff's method and consequently computed forced convection heat transfer and natural convection flows in both planar and annular geometries. Comparisons with experimental data have been impressive.

The Deardorff-Schumann approach uses artificial boundary conditions to represent the physics of the regions closest to the wall. Since much of the interesting and important physics of wall-bounded flows occurs in these regions, the Stanford group felt it important to simulate this region as exactly as possible; no-slip boundary conditions were used. Moin et al. (1978) demonstrated the feasibility of this approach and Moin and Kim (1981) refined the method so that it can be used to study the physics of turbulent flows in the vicinity of walls. They used 64 x 64 x 128 grid points and examined the structure of the flow in considerable detail. Their calculations agreed well with experimental data on the mean velocity profile and higher-order statistical correlations. They showed, through a computer-generated motion picture, that the computed flow field displays the streaks, bursts, sweeps, and ejections observed in laboratory experiments. A major portion of the LES effort in the engineering community is directed at the turbulence structure in wall-bounded flows.

Recently, the group at Electricite de France has applied LES to flows in geometries more complicated than any considered previously (Baron, 1983). The grids used are coarse, relative to the size of the eddies in the flow, but satisfactory results appear to have been achieved.

b.   Impact on Turbulence Modeling

LES is currently too expensive for engineering design use; simpler models are used for this purpose. These include integral methods and, to an increasing degree, two-equation models. The increasing sophistication of these models requires a considerable body of quality data for the establishment of their internal constants. Such data are expensive to acquire; in some cases, experimental techniques either do not exist or are not sufficiently accurate. This creates a gap which can be filled in part by LES; this role has long been on the agenda of LES workers. Some success has been achieved.

Using either FTS or LES it is possible to compute both the value of a quantity that must be represented by first- or second-order closures, as well as its model representation. By comparing these, it is possible to gauge the validity of the model and to estimate the constants appearing in it. For homogeneous flows, considerable information relating to Reynolds stress models has been obtained by Rogallo (1981), Feiereisen et al. (1981), and Shirani et al. (1981). The fluctuating pressure is particularly difficult to measure, and there are little accurate data about the terms that contain it—e.g., the pressure-strain correlations. These terms are usually modeled in two parts, one associated with the mean velocity field (called the rapid terms) and a second deriving strictly from the turbulence (the slow terms). Using FTS, these authors showed that (at least for low Reynolds numbers) the Rotta model for the slow terms is not very accurate. These models also assume that the dissipation is isotropic (see Eq. 3.1); this is found not to be true in these flows. However, when the anisotropic component of the dissipation and the slow pressure-strain term are combined, the model actually works fairly well. Tables 1 and 2 give the model constants for the different tensor indices; if the model were correct, the values for each index would be the same, and greater than 2. Models for the rapid pressure-strain do not fare well at all. Table 3 shows how unsatisfactory the results are; attempts to find improvements were unsuccessful. Therefore, either different models for these terms or a different approach to modeling is needed.

Shirani et al. included a passive scalar in their work and made the kinds of tests described above with similar results. The unique aspect of this work was the testing of several popular turbulent Prandtl number models. All were found lacking in quality; Figure 10 shows a typical test. They suggested a

new model which their tests indicated to be much better than the others;
Figure 11 shows these results. This new model has not yet been tested in
simulations of flows.

Less model testing has been done for inhomogeneous flows. Here one needs
to average LES results over homogeneous directions and, possibly, over time.
One can compute values of the model parameters as functions of the
inhomogeneous coordinate and the tensor indices. Models assume these
parameters to be constant; if they are found not to be constant, this is
evidence of weakness of the model.

Schumann and his co-workers have done much of the model testing work for
wall-bounded flows; they considered mixing-length, two-equation, and Reynolds-
stress models. They found that these models are not as accurate as had been
hoped. The current generation of such models is probably not accurate enough
to be used in engineering design work without tuning to the particular flow or
region of the flow. Schumann's group tested heat transfer models in many of
their simulations; they concluded that they are no better than those for
momentum transfer.

Riley and Metcalfe have tested Reynolds stress models for free shear
flows. Again it was found that the quality of the models left something to be
desired.

4.2 Future Directions of Large-eddy Simulation in Engineering

a. Advances in computer technology

The preceding sections show that while much has been accomplished in LES,
much remains to be done. Since LES requires considerable computer resources,
future directions will be largely determined by trends in the development of
large computers. The supercomputer projects sponsored by the governments of
the U.S. and Japan have been well publicized. Fluid dynamics computations
including engineering, meteorology, and oceanography will undoubtedly consume
a large fraction of the resources of these machines. We therefore anticipate
a large step forward in the use of LES in the next five years.

VLSI technology is making it possible to build chips with ever-increasing
numbers of circuits. This technology already dominates fast computer memory
applications and is becoming an important factor in secondary memories. In
just over ten years since the introduction of the first four-bit micro-
processor, we have seen progress through eight- and sixteen-bit systems to

Table 1

Fitting function: $f = d \left(\dfrac{SL}{q}\right)^a (1+bM^2) (Re_\lambda)^d$

Indices	c_1
$i = 1, j = 1$	1.114 ± 0.723
$i = 2, j = 2$	1.730 ± 0.899
$i = 3, j = 3$	0.680 ± 0.583
$i = 1, j = 2$	1.559 ± 1.090

Table 1. The parameter c_1 obtained by fitting Rotta's model for the "slow" part of the pressure-strain correlation to data obtained from full turbulent simulation of homogeneous shear flow. A correct model would yield a parameter which is greater than 2.0 and independent of the tensor index. From Feiereisen et al., 1981.

S = mean shearing rate

q = rms turbulent velocity

L = integral scale

M = turbulence Mach number

Re_λ = Reynolds number based on Taylor microscale

Table 2

Rotta Term with Dissipation Anisotropy $(\phi_{ij} - 2\epsilon d_{ij})$

Indices	c_1
$i = 1, j = 1$	2.886 ± 0.722
$i = 2, j = 2$	3.727 ± 0.824
$i = 3, j = 3$	1.719 ± 0.921
$i = 1, j = 2$	3.035 ± 1.122

Table 2. The parameter c_1 obtained when the anisotropy of the dissipation is included in the model tested in Table 1. Considerable improvement is noted. Source: as in Table 1.

Table 3

Fitting function: $f = d \left(\dfrac{SL}{q}\right)^a (1+bM^2) (Re_\lambda)^c$

Equation	A_2
$i = 1, \ j = 1$	0.324 ± 0.061
$i = 2, \ j = 2$	-0.134 ± 0.052
$i = 3, \ j = 3$	0.289 ± 0.088
$i = 1, \ j = 2$	0.198 ± 0.029

Table 3. The parameter A_2 obtained by fitting a commonly used model of the rapid pressure-strain correlation to full simulation data. Source: as in Table 1.

$$P = \left[1.170 + (0.837 \, Pe_T)^2 \, (1 - e^{-\frac{1.53}{0.547 \, Pe_T}}) \right]^{-1}$$

r.m.s. error = 15%

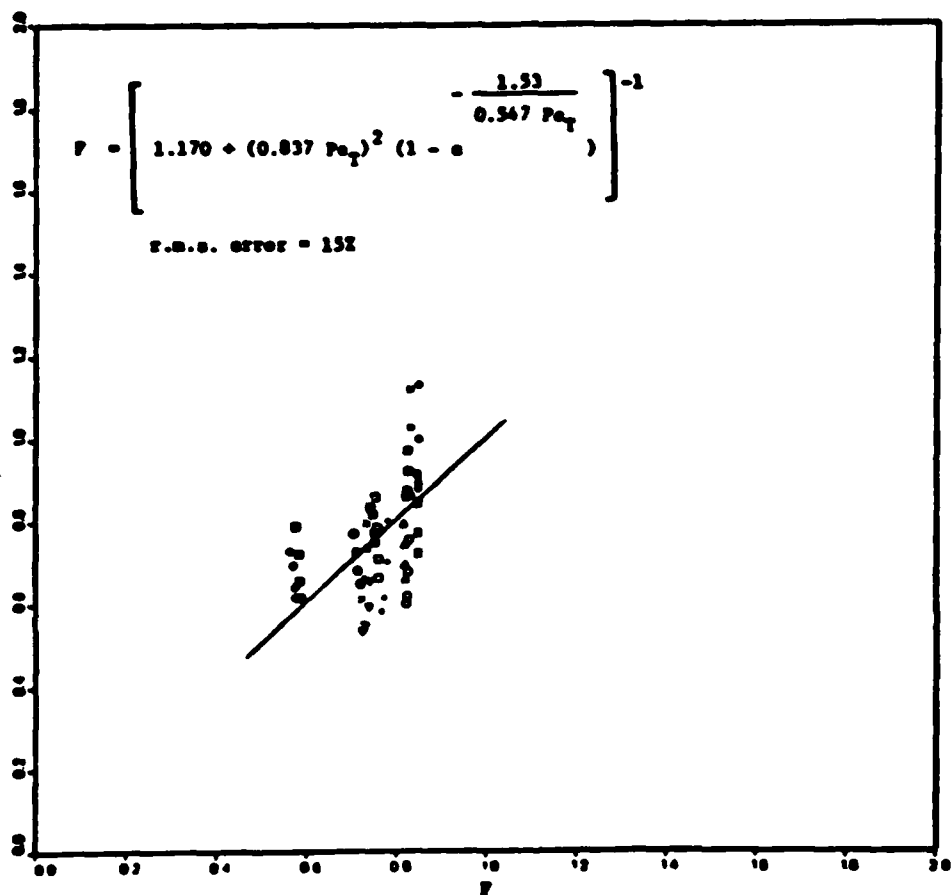**Figure 10.** Test of a turbulent Prandtl number model (parameterization); the turbulent Prandtl number is the ratio of the turbulent diffusivities for a passive scalar and momentum. The exact value obtained from a full simulation is plotted against the model value; the line was obtained by least squares fitting. The model does not appear to produce the correct trend. From Shirani et al. (1981).
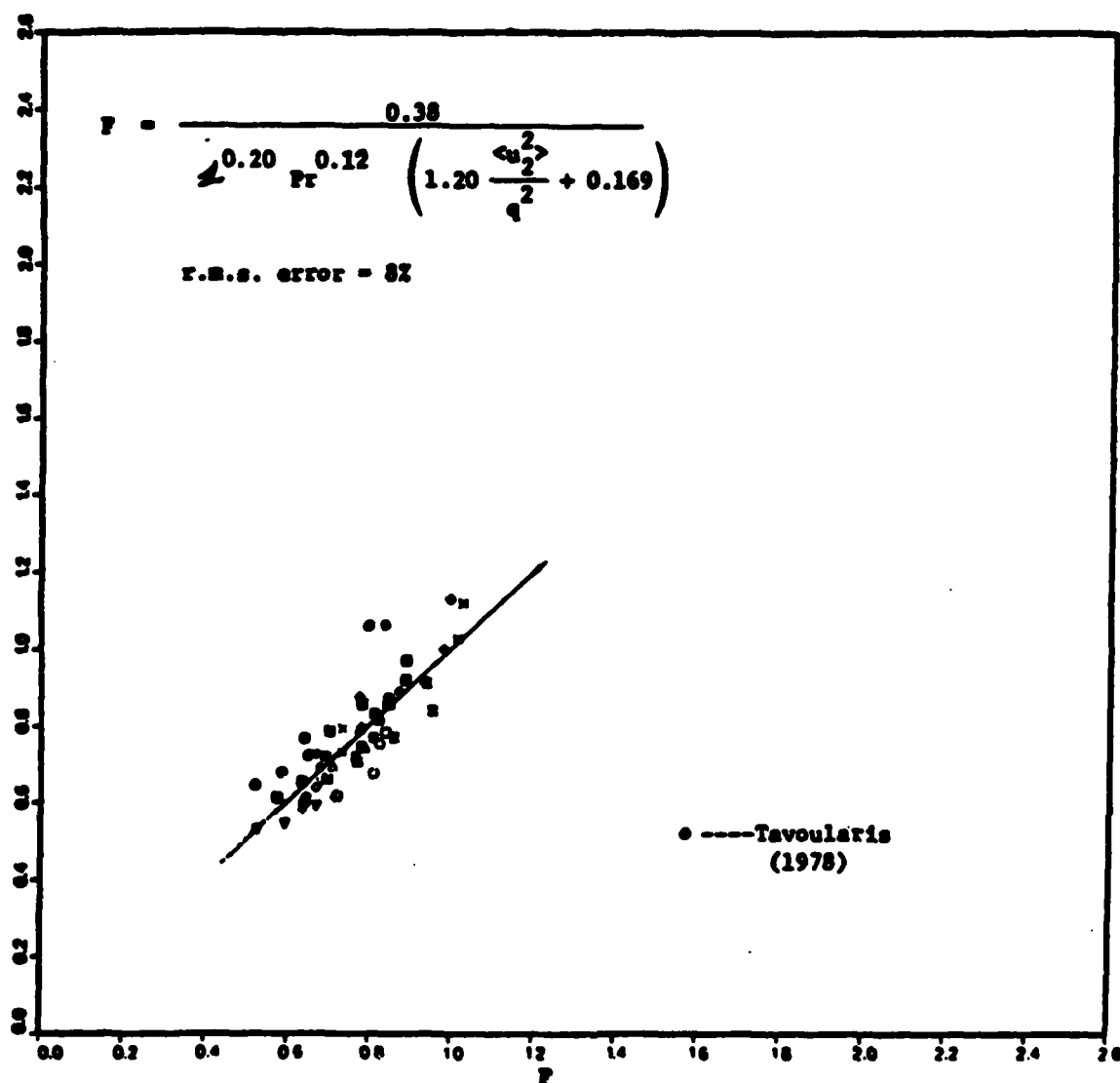
Figure 11.   Test, similar to that of Figure 10 for a new model proposed by Shirani et al. Improvement is clear, although the new model still leaves something to be desired. Source as in Figure 10.

thirty-two bit microcomputers. The current generation of chips makes it feasible to build a desktop computer which matches the mainframe of ten years ago in both computation speed and memory. When these chips are used in clever architectures, significant decreases in the cost of making a given computation can be expected. Again, there are important consequences for LES that we will consider next.

b.   LES on supercomputers

The present generation of large computers--the CRAY X-MP and the CYBER 205--are capable of approximately 100 million floating point operations per second and have 1-4 million words of fast memory. In the next few years, machines with ten times the power in both speed and memory are expected to become available. Machines with still another order of magnitude in speed (with as yet unspecified memory sizes) may become available not long after that, say in five years. Because these machines will cost as much as the present large machines, access to them will remain restricted to a small number of users. They will, therefore, be research machines and the tasks assigned to them will likely represent the natural extensions of current LES work.

Work on homogeneous turbulence will continue. The new machines will make it possible to use grids as large as 256 x 256 x 256 and, in a few cases, 512 x 512 x 512. One will finally be able to simulate flows at the Reynolds numbers of the experiments, including cases with a clearly defined inertial subrange. Since most applications flows have high Reynolds numbers, this will permit the study of subgrid-scale modeling under conditions close to those that one really wishes to simulate. Also, it may become possible to study sheared and strained turbulence for distortion times long enough to answer questions that have perplexed turbulence theorists. Thus, the new machines should lead to exciting advances in the state of turbulence theory.

The new machines should provide the capability of simulating free shear flows and some wall-bounded flows from the inception of instability to the fully developed turbulent state. This will permit the study of various perturbations on the initial stages of free shear flows; many technological applications require the ability to do this. Sound generation by turbulent flows, which can be dealt with crudely at the present state of the art, will be open for investigation. We will be able to simulate spatially developing free shear flows and study the pressure-feedback effects that have been difficult to look at in the laboratory.

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Combustion is an area of great and obvious technological importance.
Application of LES to combusting flows has been slow in coming for several
reasons. First, since chemical reaction requires mixing at the molecular
level, the small scales of reacting flows must be treated accurately. When
this is coupled with the necessity of carrying additional equations
representing the conservation of each chemical species and the notoriously
stiff equations for the chemical kinetics, one sees that the task is
formidable. Nevertheless, the new generation of supercomputers should make it
possible to begin work on the simulation of turbulent combusting flows. The
potential in this area is enormous.

For wall-bounded flows, the new generation of computers will allow full
simulation of turbulent channel flow and the flat-plate boundary layer. A by-
product will be the possibility of fully simulating laminar-turbulent
transition; this opens up many opportunities. It will also be possible to add
other phenomena (for example, unsteadiness and adverse pressure gradients) to
boundary-layer flow. This will lead to a new way of studying and developing
practical turbulence models.

c. LES in industry

Just as the coming generation of supercomputers will open up new areas of
LES research, new VLSI technology will make machines equivalent to the present
generation of supercomputers much cheaper and therefore much more widely
available. There may be instances in which engineers will choose LES as a
tool for final checking and testing of designs. As with any other new method,
there will first be exploratory investigations to test whether the idea is
sound and to refine the method. If these work out, there should then be a
slowly increasing use of LES as an applications tool.

LES may find early application in flows that are inherently three-
dimensional and time-dependent. Traditional turbulence models for such flows
are based on ensemble averaging. On the other hand, a three-dimensional,
time-dependent solution may be either an ensemble-average calculation or a
large-eddy simulation. Which should one choose? The answer depends on the
questions one is trying to answer. As an example, consider the in-cylinder
engine flow. Some questions, such as the pressure history through a cycle
and, perhaps, the choice of optimum spark timing can be answered with an
ensemble-average model. Others, such as the prediction of misfire, probably
require analysis of individual cycles via LES. Operationally, the major

difference between the two approaches can be simply the length scale appearing in the turbulence model; otherwise the same code can be used in both approaches!

There are many free shear flows of technological interest, including combusting flows. In this area, the future of LES is not yet clear; many research issues need to be resolved before we can contemplate using LES in such applications. Development needs here include a method for producing inflow conditions appropriate to LES; accurate boundary conditions for the computational outflow surface; and, finally, a method for dealing with the rapid growth of length scales in free shear flow, i.e., a method which adapts the grid size to the local eddy size. These seem to be the primary issues needing attention in the next few years.

Similar issues enter in wall-bounded flows. Spatially developing wall-bounded flows will require methods of dealing with the inflow and outflow boundaries. These flows are less turbulent and less rapidly developing than free shear flows, so the problem is not one of scale growth, but rather one of considering a sufficiently large part of the flow while using a grid small enough to capture the important eddies. To be able to do this at Reynolds numbers of technological interest, it will be necessary to eliminate the layers closest to the wall from consideration. This requires artificial boundary conditions of the type used by Deardorff and Schumann. First, the accuracy of these models needs to be checked and new models developed. We believe that this can be done by using LES at relatively low Reynolds numbers. Many phenomena which occur in boundary layers in applications should also be studied; these include heat transfer, blowing, suction, curvature, and rotation. All of these effects can be studied in geometrically simple flows.

CHAPTER FIVE
LARGE-EDDY SIMULATION: AN ATMOSPHERIC VIEW

Large-eddy simulation has proven useful in a number of meteorological applications, ranging from boundary layers to severe convective storms. The spatial resolution of an LES model is very fine, by meteorological standards, ranging from perhaps 100-300 m in PBL applications to typically 1 km in cloud simulations. As in engineering applications, the intention is that this cutoff scale should lie within the inertial subrange, so that the unresolved eddies are primarily dissipative and relatively simple to parameterize. The large-scale turbulence, which does the bulk of the turbulent transport in the PBL and is responsible for severe-storm evolution, for example, is resolved explicitly.

The major strength of the LES technique, clearly, is its ability to resolve the mean and the largest-scale turbulent fields, with minimal reliance on closure models of unknown validity. As a result, the credibility of LES results tends to be relatively high, which is very important in boundary-layer meteorology where definitive observational data are scarce and expensive, as we saw earlier.

5.1 Boundary-layer Studies

In Deardorff's first LES studies of the boundary layer (summarized in Deardorff, 1973), he used a rigid lid and simulated neutral and convective cases. He found that stable stratification eliminated the largest eddies and forced the turbulence to be subgrid scale, and so reported no results on the stable PBL. While in principle a grid-adjusting scheme should allow simulation of the evolution of a stable PBL by changing the grid size with time, we know of no published results.

Deardorff later replaced the rigid lid with a capping inversion layer, and in two 1974 papers presented the results of an LES study of day 33 of the Wangara experiment in Australia. His mean-field results (paper 1) agreed well with observations, but the more remarkable aspect of his study was the detail

it revealed about the turbulence structure (paper 2). These turbulence results far outstripped the observations. He presented mean profiles, second-moment budgets, and even a comparison of calculated pressure covariance profiles with current parameterizations.

Sommeria (1976), working with Deardorff, extended this LES model to include most of the physical processes occurring in a moist boundary layer in the absence of precipitation. Refinements included a water cycle, with cloud formation, and infrared radiative cooling in clear and cloudy conditions. Sommeria and LeMone (1978) used a further improved version of this model to simulate conditions in the fair-weather PBL over the typical ocean observed in the 1972 Puerto Rico experiments. The comparisons of second-order turbulence moments, the PBL roll-vortex structure and the cloud structure were generally satisfactory. Later, Nicholls et al. (1982) used this model to simulate a fair-weather marine boundary layer in GATE and found quite encouraging agreement with the observations.

Deardorff (1980) presented results from an LES study of stratocumulus-topped mixed layers. He was able to study the nature of the cloud-top radiative cooling which helps to drive the mixed layer and to develop an expression for the entrainment rate in the presence of variable stratocumulus. Again, he presented details on the turbulence field which are far beyond our experimental reach. Lamb and Durran (1978) used the velocity fields from Deardorff's LES work, plus an innovative numerical scheme, to infer eddy diffusivities for continuous-point-source diffusion in a convective PBL. While the diffusivity did scale with w_*z_i, as expected, it also depended strongly on the height of the pollution source; this contradicts the assumptions underlying conventional Gaussian-plume models.

Wyngaard and Brost (1984) studied scalar transport in a convective PBL with Brost's LES model, which was patterned closely after Deardorff's. They studied what they called "top-down" and "bottom-up" diffusion, or the transport of a scalar whose flux is zero at the PBL bottom, but nonzero at the top, and vice versa. They found that the bottom-up eddy diffusivity was more than twice as large as that in the top-down case, which indicates that current K-closures are fundamentally wrong.

Moeng (1984) has produced a new LES code for PBL studies; it uses pseudo-spectral techniques in the horizontal, which are computationally more efficient than finite differences. She has recently verified and extended the

Wyngaard-Brost results and has completed a study of the statistics and dynamics of the top-down and bottom-up scalar concentration fields in a convective PBL (Moeng and Wyngaard, 1984).

This productive LES work could be profitably extended in a number of ways. The influence of differential (i.e., height-dependent) mean advection and baroclinity on mean profiles, which can be important on the mesoscale, could be studied and parameterized through LES. The influence of variable surface properties and cloud cover on PBL structure could likewise be studied. A pressing need is the extension to stable stratification and the nocturnal PBL, whose physics remain elusive. LES should also be used to study the PBL during the morning and evening transition periods, which are also poorly understood. Other extensions include the PBL in near-neutral conditions, and over complex terrain.

5.2 Diffusion Studies

LES velocity fields have served as the basis for some landmark diffusion studies. In such applications one assumes that the pollutant concentration is not so large that it alters the radiation fluxes through the PBL and, hence, affects the PBL dynamics. In most applications this assumption is valid. Thus, Lamb's (1982) diffusion calculations for a convective PBL used the output of Deardorff's (1974) LES runs.

In his 1982 review paper, Lamb described a method for using an LES velocity field to calculate dispersion. In his notation, $X_i^m(t)$ denotes the vector position at time t of the particle (assumed neutrally buoyant) released at (x_m, y_m, z'); i.e., $X_i^m(t) = x_i(x_m, y_m, z', t)$.

By definition,

$$\frac{d}{dt} X_i^m = \hat{u}_i(X_i^m(t),t) + u_i'(X_i^m(t),t), \qquad (5.1)$$

where $\hat{u}_i$ is the velocity field resolved by the LES model and u_i' is the unresolvable (subgrid-scale) field.

Lamb's process for determining u_i' is described in detail in his 1981 paper. Briefly, his approach is to delineate a set of functions whose set-mean statistics are identical with the known statistics of u_i', and then to pick members from this set at random for each of the M release points. For

example, the subgrid-scale parameterization scheme of the LES model provides an estimate of the local mean square of u_i'. We also know that u_i' is approximately isotropic, that its wavenumber components lie within the inertial subrange, and we can make educated guesses of its temporal autocorrelation and integral time scales. This information does not uniquely specify u_i', but does serve to constrain the range of choices.

Lamb generated his u_i' through the algorithm

$$u_i'(X_i,t) = \alpha u_i'(t - 2\Delta t) + \beta u_i'(t - \Delta t) + \gamma \rho_i, \qquad (5.2)$$

where ρ_i is a computer-generated, isotropic random vector with zero mean and variance

$$\overline{\rho_i^2} = \frac{2}{3} E, \quad i = x, y, \text{ or } z, \qquad (5.3)$$

where E is the subgrid-scale turbulent kinetic energy at x_i,t, from the LES model. Lamb also showed that the parameters α, β, and γ in (5.2) must satisfy two constraints.

Lamb (1982) showed that his scheme gave good agreement with both atmospheric and laboratory convection tank observations for neutrally buoyant cases. He has also extended his calculation technique to buoyant sources and found that source buoyancy has surprisingly large effects. Much more work remains to be done on source-buoyancy effects, however.

5.3 Computational Details

a. Integration techniques

Integration techniques available to the LES modeler include finite-difference schemes, spectral and pseudospectral methods, and finite-element and interpolation schemes. Pielke (1984) has recently described these techniques and considered their application to mesoscale problems. We will briefly summarize them as they bear on LES models for transport and dispersion in the PBL.

Finite-difference schemes. This approach involves approximating the time and space derivatives by one or more terms in a Taylor series expansion. In meteorological applications, the expansions have generally been limited to first or second order in time and second or fourth order in spatial

derivatives. Care must be taken in the design and use of finite-difference schemes such that they remain linearly, computationally stable. Also, casting of the spatial derivatives in the so-called flux-conservative forms (i.e., Arakawa, 1966) will prevent the development of nonlinear instability due to the accumulation of energy at the grid truncation scale (Δ). Using terrain-following coordinate transformations, the schemes can be applied to quite complex terrain mappings, and they are adaptable to a variety of lateral boundary conditions.

Spectral and pseudospectral methods. The spectral method involves the transformation of the governing equations through the use of global basis functions, such as a truncated Fourier series or spherical harmonics (the latter being useful in hemispheric or global atmospheric models). The pseudospectral method involves performing a part of the required operations-- say those involving the horizontal coordinates--in spectral space, and then transforming to finite-difference Cartesian space for vertical advection and other physical processes. For the same number of degrees of freedom, spectral methods are more accurate than finite-difference schemes, provided that the flow field is sufficiently smooth (well-resolved) (Fox and Deardorff, 1972; Orszag, 1971; Machenhauer, 1979).

Finite-element methods. The finite-element technique differs from spectral or pseudospectral techniques in that a local rather than a global basis function is employed. Examples of such basis functions are the Chapeau or linear-basis function (Long and Pepper, 1976) and the quadratic function (Pinder and Gray, 1977). For the same number of degrees of freedom as a finite-difference scheme, the finite-element method is more accurate and eliminates the possibility of aliasing energy cascading onto the truncation scale and then back into the larger resolvable scales. Furthermore, it can be readily adapted to arbitrary lateral boundary conditions and to relatively complex topography.

If the finite-element and finite-difference techniques are matched in terms of computational demands, no clear-cut advantage of one over the other has been demonstrated. Longer time steps can be used than with finite differences, although for larger values of Δt, phase errors may be introduced in the solution. Some saving in computational demands can be made by using one-dimensional basis functions in each coordinate direction, rather than using a local multidimensional basis function.

Interpolation schemes. Interpolation schemes or semi-Lagrangian schemes basically estimate the time derivative due to advection by interpolating to evaluate the advected quantity at a distance $U_i \Delta t$ from a given grid point at the time level τ. The interpolation formulas range from the bilinear (or trilinear) interpolation formula used by Murray (1970) to Mahrer and Pielke's (1978) spline interpolation formula. Interpolation techniques completely eliminate the $2\Delta x$ wave, thus preventing aliasing or nonlinear instability, and are convenient for variables which remain conserved in a Lagrangian sense (e.g., total water mixing ratio in a nonprecipitating cloud).

The above techniques have a common problem when simulating the dispersion of sharp-edged plumes of a scale comparable to the trunaction scale of the numerical operators. In such cases, positive-definite quantities (such as concentration) can become negative. This problem is frequently met in cloud modeling, where workers have resorted to various techniques to assure positive definiteness (e.g., Clark, 1979; Tripoli and Cotton, 1982). Interpolation schemes and spectral techniques are particularly troublesome in this regard, as are finite-element techniques and some finite-difference methods such as leapfrog/quadratic conservative space operators. There are finite-difference techniques under development which can minimize this problem at additional numerical cost (Smolarkiewicz, 1983, 1984).

b. Evaluation of pressure

The pressure field in an LES model must be evaluated nonhydrostatically, and there are currently two approaches. One, used by Deardorff (1972) and cloud modelers such as Clark (1979), assumes the flow is incompressible. Pressure is then evaluated by taking the divergence of the equations of motion and forming an elliptic or Poisson-type diagnostic equation for pressure. Since sound waves are eliminated from the system, the time steps of explicit integration schemes are limited by slower moving internal gravity waves and advection time scales, rather than by fast moving sound waves.

The second approach, used by Klemp and Wilhelmson (1978a) and Cotton and Tripoli (1978), is to retain compressibility and to evaluate pressure by a so-called time-splitting procedure. In this procedure the terms in the equations of motion contributing to sound waves are separated from the long-time-scale terms. The sound wave generating terms and a simplified equation of continuity or pressure tendency are integrated on a small time scale which resolves sound waves, while the terms and equations governed by internal waves and advection are integrated on a time step some 10 to 30 times longer.

Neither technique for evaluating pressure exhibits clear superiority in terms of computation speed. Since the compressible part of the time-split procedure is readily vectorized, it is a fast procedure on modern super-computers. On the other hand, inversion of a Poisson equation is not a particularly efficient procedure on these computers. However, the procedure need only be exercised at 1/10 to 1/30 the frequency of the compressible, time-split calculation. Preliminary results of a comparative study among time-split compressible and anelastic nonhydrostatic models, as well as hydrostatic models by Tripoli and Tremback (Cotton, personal communication), reveal that the anelastic approximation (or incompressible approximation) has a consistent damping influence on vertical motions. In a deep convective situation the anelastic model underpredicts peak vertical velocities by as much as 30% relative to the elastic model. Thus, it appears that the greater freedom of an elastic model allows the formation of higher amplitude convective velocities. This may have significant bearing on LES model simulations of boundary-layer transport processes.

c. **Boundary conditions**

In any limited fine-mesh model, the prescription of boundary conditions at the top, bottom and sides of the domain has a significant influence on the solutions. In LES models the common approach is to employ periodic (cyclic) lateral boundary conditions (see Deardorff, 1972; 1980). The advantage of this technique is that eddies which propagate through an outflow boundary will re-enter the model domain on the inflow boundary. This allows continuous evolution of the statistics of the simulated turbulent elements, since the velocity fluctuations of eddies entering the inflow boundary will be the same as those created in the model interior and then propagated out the outflow boundary. This is only true for eddies which are fully contained within the limited domain of the model. Periodic boundary conditions can distort larger-scale eddies such as boundary-layer roll vortices, which may be only partially captured in the model domain (Sommeria and LeMone, 1978).

In LES simulations with inhomogeneities in roughness, terrain, or heating functions across the domain, it would be incorrect, for example, to advect into the upstream boundary eddies which have formed over terrain with different features. In this case it may be desirable to use open, "radiative-type" boundary conditions such as used by Klemp and Wilhelmson (1978a) or Orlanski (1981). The boundary conditions allow gravity waves generated in the

model domain to propagate freely out of the downstream boundary. The inflow
boundaries are prescribed, however. Thus, the turbulence field must evolve
from a nonturbulent inflow state; this means that the inflow boundary must be
well removed from the region of LES analyses. This is a familiar problem in
meteorological modeling and could represent a serious limitation to LES in
some applications.

The bottom boundary conditions must treat near the earth's surface the
energetics and fluxes generated by eddies smaller than the resolvable scales
of the model. The conventional approach is to use surface-layer similarity
(Deardorff, 1972). The major difficulty is formulating the similarity laws
and the subgrid-scale closure schemes such that they are compatible at the
interface between the surface layer and the model domain (Manton and Cotton,
1977).

The rigid lid used in early LES models (e.g., Deardorff, 1972) is
appropriate as long as the boundary-layer eddies do not advect near the upper
boundary and do not trigger internal gravity waves in the overlying stably
stratified free atmosphere. However, since vigorous boundary-layer eddies
perturb the overlying stably stratified free atmosphere, they are likely to
excite internal waves which can reflect their energy back into the model
domain causing perturbations in z_i and, as a result, in the boundary layer
statistics. Thus, the optimum upper boundary condition is a "radiative-type"
upper boundary condition, such as described by Klemp and Durran (1983). Such
a boundary condition allows gravity-wave energy to pass through the model top
without reflecting energy into the model interior; this can contaminate
boundary-layer statistics.

Radiative top and lateral boundary conditions are most desirable when the
terrain is irregular and/or the overlying free atmosphere is quite stable and
the winds are strong.

d.   Closure schemes

LES models are intended to resolve the energy- and flux-carrying
turbulent eddies explicitly, and therefore allow the use of a simple subgrid-
scale closure model. Most of the subgrid schemes now in use have their roots
in the second-moment conservation equations for the subgrid-scale
turbulence. Deardorff (1973) has given a lucid description of this topic.

Some insight can be gained from theory here if the gridscale is
sufficiently far into the inertial range that one can assume local isotropy.

Lilly's (1967) early calculations of this type provided much of the closure foundations for Deardorff's LES models.

Attempts have been made to carry a "full" set of subgrid-scale moment equations (Deardorff, 1974a), but this is computationally demanding. Later engineering LES experience, based on comparisons of LES and full turbulence simulations, suggested that these more sophisticated subgrid-scale closures did not actually represent the unresolved dynamics appreciably better. Thus, current atmospheric LES models usually carry only a subgrid-scale turbulent kinetic energy equation to provide a subgrid velocity scale. The subgrid length scale is the grid spacing Δ (which need not be uniform throughout the domain), and these two parameters together with standard turbulence scaling arguments (Tennekes and Lumley, 1972) provide the subgrid-scale closures.

e.   Domain, resolution, and computer time

The Colorado State University Regional Atmospheric Modeling System (RAMS) is useful as a guide for obtaining estimates of LES model timing on modern class-6 computers, such as the CRAY-1A. For a model having resolution of $\Delta x = \Delta y = 150$ m and $\Delta z = 50$ m and a domain of 28 x 59 x 59 points (1.4 x 8.8 x 8.8 km), the ratio of simulated time to computer processing units (CPU) is $\approx 1/3.5$. Thus, a two-hour simulation plus one-hour start-up time will require 10.5 hours CPU-CRAY. However, this represents only one independent realization. To obtain statistically significant ensemble-averaged data, several realizations are required. This may increase by a factor of 10 the CPU time needed for a "representative" LES ensemble-averaged result. Unfortunately, a horizontal domain length of 8.8 km is not large enough to accommodate 10 km mesoscale eddies, which (at least in some circumstances) are dominant contributors to the horizontal wind variance.

To increase the horizontal domain to 15 km and maintain a practical computational level, one is forced to increase the grid truncation scale. For example, a 28 x 59 x 59 point domain covering 15 km in the horizontal and having resolution of $\Delta x = \Delta y = 250$ m and $\Delta z = 100$ m will have a ratio $= \dfrac{\text{simulated time}}{\text{CPU}} = 1/2$. Thus, a single two-hour simulation plus one-hour start-up time will require six hours CPU-CRAY.

f. Computer Expectations

The future growth of LES studies of the PBL depends heavily on two major developments. The first is improvements in subgrid-scale closure theory which will permit coarser-resolution simulations. The other is expanded computer power.

The speed-domain estimates we gave above were based on the CRAY-1A computer system. This system has 10^6 words of central memory and is capable of speeds in the range of 10 to 140 million floating point operations per second (mflops). Normally, Fortran-coded problems operate over the speed range of 30 to 85 mflops. The CYBER 205 has a slightly broader range of computational speeds with most Fortran-coded problems running on the low end of the CRAY range. The central memory available on the CYBER 205 ranges from 2M words full 64-bit memory to 4M half precision words. CRAY Laboratory is currently marketing the CRAY X-MP, a multiprocessor, vector-based computer; however, software for linking the multiprocessors is not available. By the end of 1984 we may expect this system to be operating on Fortran codes in the range 120 to 400 mflops.

By 1986 several major advances in supercomputers can be expected. These could come from one of several U.S. vendors or Japanese supercomputers looming on the horizon.

It is likely that computers operating on Fortran-coded problems will operate in the range of 700 to 1000 mflops, or slightly greater than a factor of 10 faster than class-6 computers. The greatest advances are expected to be in the area of high-speed memory; if its cost goes down and the speed of the computers goes up, while input/output (I/O) speeds remain the same or show modest improvements, we can expect vendors offering computers with as much as 256 M 64-bit-word memories.

Thus, by 1986 it should be possible to operate LES models well into the meso-γ domain (i.e., 10-25 km) with resolution $\Delta = 50$ m and at speed equal to or faster than real time.

Figure 12 is a plot of past and projected computer speed and memory. The historical data are adapted from Chapman (1979), while the projected data are mid-range values of the estimates in this report.
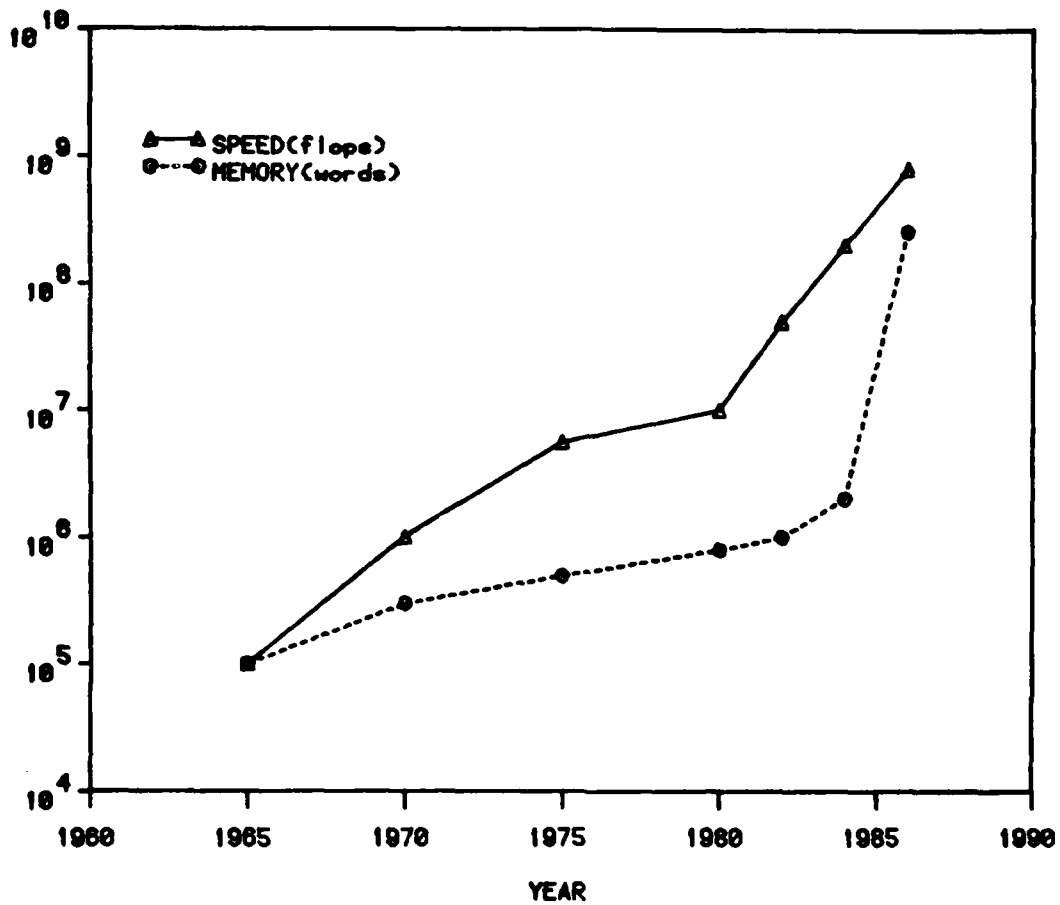
COMPUTER HISTORY

Figure 12.   Past and projected computer speed and memory. Historical data from Chapman (1979); projected data are mid-range values from this report.

5.4 Some Limitations of LES

The various applications of LES to problems in small-scale meteorology over the past 15 years have also revealed some limitations of the technique.

The PBL, by its nature, tends to be confined from above by an inversion whose stable stratification reduces eddy sizes in the turbulence at the PBL top. The lower surface also acts to reduce eddy sizes in its vicinity. As a result, LES resolution is worst near PBL bottom and top, where important transfer processes can take place. Transfer at the bottom is well understood from surface-layer experiments and, can probably be adequately parameterized for most problems, but the same is not true at the top. The interfacial layer which buffers the convective PBL from the free atmosphere is still largely a mystery in its dynamics, and it is not clear that it can easily be studied with LES. Increasing the vertical resolution might not solve the problem, because one would expect the three-dimensional nature of turbulence to dictate a reduction in horizontal grid size as well.

There is also evidence that eddies of scale larger than typical LES domains can be quite important in small-scale meteorology—i.e., that the domain size does not often fall in a "spectral gap." For example, Sommeria and LeMone (1978) and Nicholls et al. (1982) found that their LES results underestimated the variances of specific humidity and horizontal wind, because the horizontal scales contributing the most to these variances was of the order of 10 km, larger than the LES domain size.

The exclusion of eddies larger than the domain size is a fundamental limitation of the LES technique, because the atmosphere contains energy in the horizontal component of turbulence at all scales, limited only by the circumference of the earth. This lateral "turbulence" is known as long waves to global forecasters, as traveling high and low pressure systems to synoptic meteorologists, as frontal zones and squall lines to regional meteorologists, as cloud complexes to cloud physicists, as convective eddies and longitudinal roll vortices to planetary-boundary-layer researchers, and as small-scale isotropic turbulence to surface-boundary-layer specialists. Lilly (1983) points out that much more mesoscale energy exists than can be predicted by the decay of geostrophic turbulence, and reasons that some of this larger-scale turbulence is produced by up-scale transfer from generation by gravity waves and stratified turbulence. Figure 13 is an example of a horizontal energy spectrum which confirms that no spectral gap exists.

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Because of this exclusion of eddies larger than the LES domain size (d), the standard deviation of the lateral distribution of pollutants, σ_y, calculated using the LES model output, will grow in proportion to the square root of time at larger travel times. However, atmospheric measurements show that σ_y is proportional to travel time, for travel times out to several days (Gifford, 1982b), as shown in Figure 14. One must recognize this limitation and interpret diffusion results in terms of the time and space scales imposed by the domain of the LES model.

The LES approach is also inherently expensive, particularly in dispersion applications, because it yields tremendous detail which can only be made statistically meaningful by averaging over time and over several runs. For example, a single LES run and its associated diffusion calculation might correspond to a one-hour experiment in the atmosphere. We know from experience that stable statistics approaching the true ensemble average ones are likely only if this exercise is repeated 10 to 100 times. At current computer rates, therefore, it might cost on the order of $100,000 to produce a reasonably stable average with LES techniques. This is very expensive compared to other modeling techniques, but should properly be compared to the costs of field measurements.

Boundary conditions can also be troublesome. Periodic lateral boundary conditions are often used, as we discussed earlier, but are not appropriate for many problems, including some in dispersion. Sommeria and LeMone (1978) found some evidence that their use of periodic lateral boundary conditions influenced the evolution of clouds in their model. Open boundary conditions are an alternative, but are difficult to implement properly when one does not know the behavior outside the domain.

Numerical techniques need to be developed for the explicit simulation of the dispersal of sharp-edged plumes while maintaining positive definiteness of concentration and preserving the sharp gradients.

Diverse and important PBL phenomena are triggered by local structure at the lower boundary. Spatially varying albedo, surface roughness, surface elevation, and other properties can all influence the PBL flow above. Proper representation of these influences in LES, in a region where much of the structure is subgrid scale, remains a challenge for future workers. Perhaps some of the innovative nested-grid techniques of small-scale meteorology (e.g., Clark and Farley, 1984) could be used.
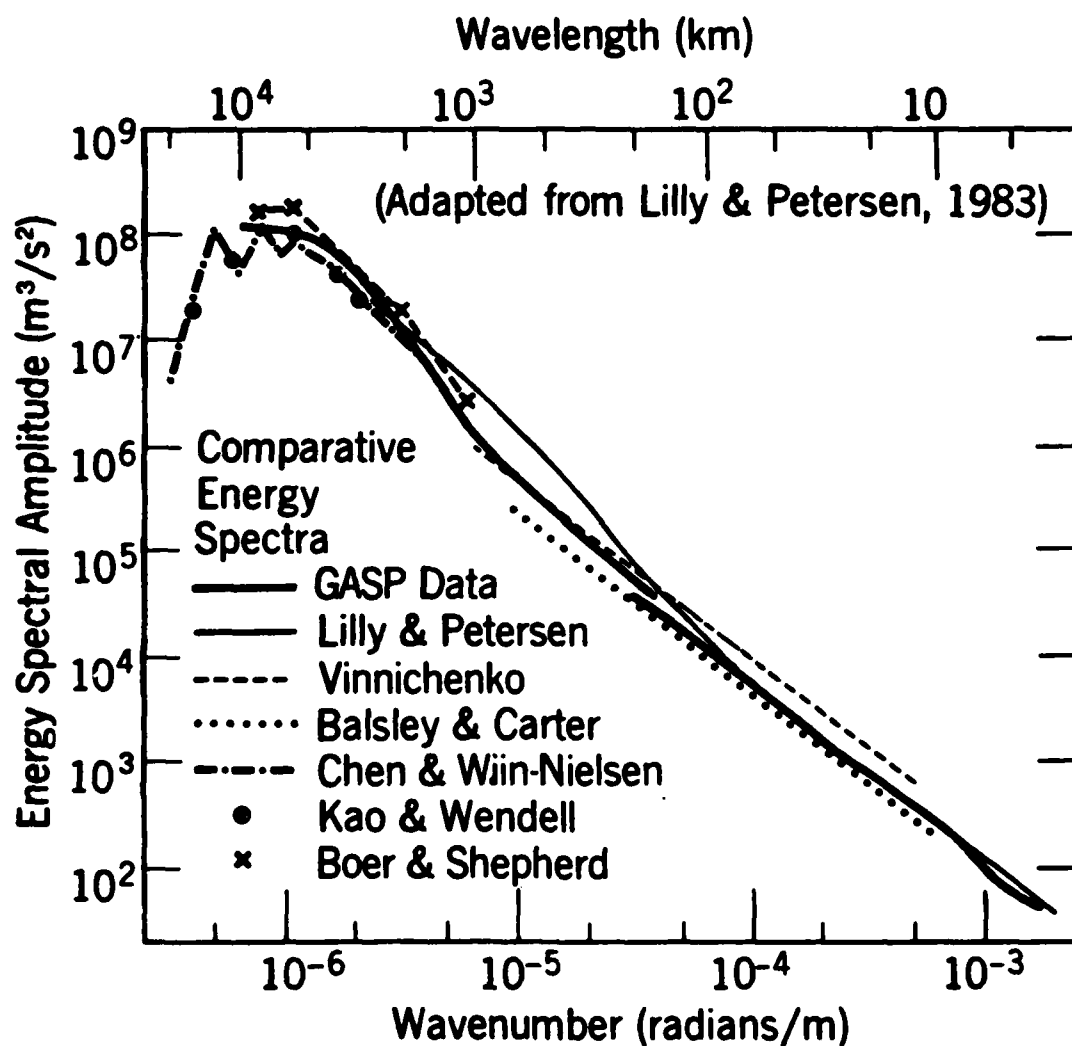
Figure 13. Horizontal energy spectra over the wavelength range from about 5
km to the earth's circumference. The Balsley-Carter and
Vinnichenko spectra were originally produced from time records,
while the Nastrom-Gage and Lilly-Petersen data were obtained from
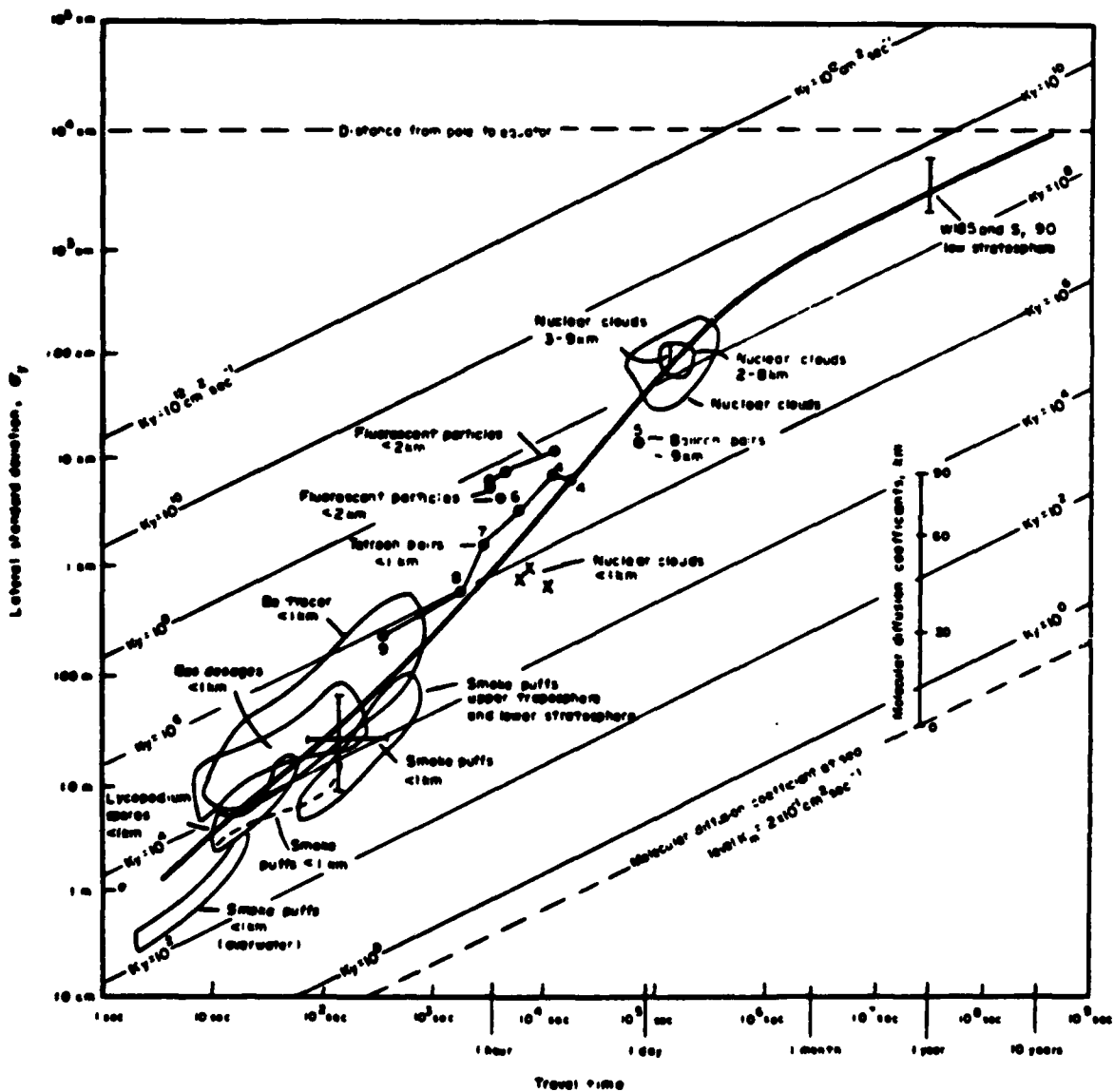jet aircraft records. From Nastrom and Gage (1984).

Figure 14.   Summary of data on horizontal atmospheric diffusion, from Gifford (1982a). The solid curve is empirically fit.

CHAPTER SIX
ROLES FOR LES IN PBL RESEARCH

Some major points regarding the current status of PBL research emerge from our previous chapters. Briefly summarized, these are

1. Inherent uncertainty is a major complication in PBL research, strongly influencing both experiment and modeling. There have been few attempts to generalize models to include prediction of inherent uncertainty; in general this remains a challenge for the future. Developing a new generation of models which predict inherent uncertainty along with the means requires a broader, more reliable PBL data base than now exists.

2. Because of their cost, difficulty, and limitations, field experiments cannot be relied on to provide the improved PBL data base necessary for the next generation of models. However, this data base would benefit greatly from measurements in carefully designed laboratory experiments which simulate certain aspects of the PBL.

3. LES experiments also have the potential of contributing substantially to this data base through "field programs" on the computer. Although LES has some limitations in PBL applications (e.g., loss of eddies larger than the domain size, poor resolution near bottom and top, difficulties with boundary conditions), the advances which we expect in supercomputers over the next several years should ease these somewhat. LES experiments also have some unique advantages, such as allowing the experimenter to control individual variables in order to study their effect on the flow.

In assessing possible roles of LES in future PBL research, our committee considered carefully the recent history of LES in small-scale meteorology (Chapter Five), but also weighed heavily its role in engineering fluid mechanics (Chapter Four). <u>LES has been very productive in these engineering research applications, and our committee feels that LES can become as</u>

important an influence in PBL research. This chapter discusses some of the roles that we feel LES can play in the PBL research of the future.

6.1 LES and Inherent Uncertainty

Inherent uncertainty--the inevitable difference between the behavior of a PBL field in a given realization and its most likely (i.e., ensemble-average) behavior--is particularly important in dispersion applications. Today, the dispersion modeling community tends to agree that a prediction of inherent uncertainty can be just as important as a prediction of mean values.

In dispersion problems, inherent uncertainty involves the statistics of concentration fluctuations. As we discussed in earlier chapters, these are rarely measured in the atmosphere; most existing data come from laboratory experiments. LES models have the potential of contributing substantially here, because an ensemble of LES-predicted realizations of a given dispersion problem would yield both the mean behavior and the inherent uncertainty. Thus, it should be possible, for example, to use LES to generate many of the probability distribution functions needed in dispersion applications.

6.2 LES and Data Bases

Large-eddy simulation can, in principle, yield detailed data on PBL structure and processes, and as we have discussed in earlier chapters, these data have a wide variety of potential uses. We will briefly summarize what we judge to be the more important ones.

a. Profiles for integral models

As we discussed in Chapter Three, integral models have applications ranging from turbulent dispersion to heat, mass, and momentum transfer. Whatever their intended application, they are based on specified forms for certain mean profiles. Gaussian-plume dispersion models, for example, are based on the assumption that a plume from a continuous point source has a Gaussian mean profile; mixed-layer models for the PBL assume that the mean wind, temperature, and scalar mixing ratio profiles are "well-mixed," or flat. While these profile forms are traditionally based on direct measurements, LES could, in principle, be a better source of data in some cases. Lamb (1982) has discussed this approach in dispersion problems and shows how the Gaussian model can be improved with LES profiles. As another

example, Wyngaard (1984) has used LES profiles of scalar mixing ratio in the convective PBL to develop an integral model for scalar transport.

b. Studies in dynamics

The studies of severe storms by J. Klemp, R. Wilhelmson and colleagues provide excellent examples of the use of LES results to study the basic dynamics of atmospheric processes. They studied storm splitting (Klemp and Wilhelmson, 1978a,b), long-lived storms (Wilhelmson and Klemp, 1978), mature supercell storms (Klemp et al., 1981), and the early stages of tornadogenesis (Klemp and Rotunno, 1983). This illustrates that LES results, like direct measurements, can be analyzed in the context of the governing equations to yield insight into the underlying dynamics.

c. Parameterizations for higher-order-closure models

As we discussed in Chapter Three, higher-order-closure models rely on parameterizations which, for PBL applications, are not yet fully tested and verified because of the lack of suitable data on PBL structure. LES results have the potential of providing data suitable for this testing process. For example, the fluctuating pressure field in the energy-containing range is resolved explicitly in LES, so that the various pressure covariances in the second-moment conservation equations can be calculated directly; in fact, they can be separated into contributions from mean strain, buoyancy, rotation, and turbulence, as they sometimes are in second-order modeling. In this way, parameterizations for these terms could be tested, and new ones developed as needed. Turbulent transport (third-moment divergence) parameterizations could be assessed in the same way.

d. Parameterizations for meteorological models

Any three-dimensional meteorological model needs parameterizations for subgrid-scale process within and above the PBL. Like any turbulence parameterization, these are difficult to generate rationally. Thus, these subgrid parameterizations tend to be crude, although they might represent very important effects--such as the turbulent chemistry in long range transport, the turbulent dispersion on the mesoscale, or the transfer processes within individual cumulus clouds. LES can be an excellent way to generate these parameterizations.

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e.   Experiment simulation and design

Some PBL problems--perhaps ones with particularly complex physics, or
ones which are site-specific--require direct measurements, in spite of the
difficulties they entail. In such cases, in order to make best use of
resources, one needs to design the experiment carefully. We feel that LES
modeling of proposed experiments could be of considerable benefit in this
design phase.

LES could also provide meteorological test fields for the evaluation of
new remote sensing techniques, such as the method proposed by Lilly and Moeng
(1984). It uses the three-dimensional, time-dependent field of a single
(radial) component measured by a Doppler radar, plus the constraints provided
by the continuity and vorticity equations, to extract the full velocity field.

CHAPTER SEVEN

LES IN BOUNDARY-LAYER RESEARCH:
LONG-RANGE GUIDELINES

Our previous chapters make it clear that LES has been used to study a wide range of PBL problems, including turbulent dispersion. However, it is also clear that associated theoretical, computational, and experimental work needs to be done before our confidence in its performance in general PBL applications reaches the level it now enjoys in engineering shear flow applications, for example. Thus, our committee feels it is important to establish some general guidelines for long-term development of LES models for the planetary boundary layer, in order that investments in LES research can provide optimum returns.

7.1 Program Components

Our committee feels that an optimum program to develop LES techniques for application to planetary boundary layer problems, with an eventual focus (on a several-year time scale) on turbulent dispersion, should have theoretical, computational, experimental, and technology-transfer components. The progress of the NASA Ames-Stanford University coalition in developing LES models for shear flows, using this broadly based approach, has been very rewarding. Although a specific strategy for LES development is beyond the scope of our study, we will offer general guidance on a number of research issues.

a. Theory

As we discussed in Chapter Five, LES has been applied to a number of small-scale problems in meteorology over the past 15 years, including studies of PBL structure, diffusion, and severe storms. Some of these applications have been strikingly successful. Nonetheless, our committee has identified a number of important but unresolved theoretical issues associated with LES, and consequently feels that it is not yet a completely reliable, general-purpose tool for solving PBL problems.

Some of these issues relate to the parameterization of the subgrid-scale eddies; Herring (1979) has given a theoretician's view of some of the principal problems here. Some progress has recently been made for shear-flow applications, as we summarized in Chapter Four, but the optimum approach to subgrid buoyancy effects, for example, is still not clear. Possibly spectral closure theory could provide useful insights, judging from recent work (Larcheveque et al., 1980; Chollet and Lesieur, 1981).

Subgrid-scale parameterization is particularly important in dispersion applications, as we discussed in Chapter Five, since it must represent the early stages of two-particle diffusion in their entirety if the initial separation is less than the grid spacing. Lamb (1981) has made some theoretical progress here, but much remains to be done, particularly for buoyant sources.

Kraichnan (personal communication) is currently studying nonlinear systems with many modes; his intent is to develop a rational technique for calculating the system evolution by carrying only a few of the modes but using the moment constraints given by the full set. His results to date are preliminary, but give some encouraging indications that a few well-chosen modes plus a moment constraint can accurately represent the full, nonlinear system. One implication for turbulence modeling could be that a finite number of wavenumbers, distributed through the turbulence spectrum (including the inertial and dissipative ranges) might ultimately allow better predictions than the current LES approach (which concentrates the modes in the energy-containing range and does not resolve structure at larger and smaller wavenumbers).

There are also unresolved theoretical problems in the specification of lateral boundary conditions, particularly in dispersion applications. A related problem is the proper accounting for eddies larger than the LES domain size, which we showed in Chapter Five can also be very important for dispersion. Finally, there are also numerical problems in the simulation of the dispersal of sharp-edged plumes of material.

b. Computation

We showed in Chapter Four how the engineering LES community is continuing to use full turbulence simulation (FTS) as a tool for developing LES. It has been extremely valuable, for example, in testing and refining subgrid-scale parameterizations. Extending FTS to turbulent dispersion, and to stably and

unstably stratified flows, is an important and necessary step toward the optimum development of LES for PBL applications, in our view. Even though the FTS techinque is limited to low Reynolds numbers, it can give data bases all but impossible to obtain in any other way.

c. Experiment

By its nature, an LES model predicts a large array of flow properties. We feel that as many of these properties as possible should be tested against measurements from both the laboratory and the atmosphere. In Chapter Two we described a number of specific laboratory experiments which should be done in stably and unstably stratified flows. Testing against such data bases has proven to be a very powerful technique in the development of engineering LES models.

Although there are indications that the days of large-scale, intensive PBL experiments yielding vast, research-quality data bases may be past, there is a possibility that PBL experiments will be carried out during the proposed STORM program of the late 1980s. If so, we would recommend that the data be used for testing LES predictions, to the extent possible.

Ideally, atmospheric measurements for the testing of LES predictions would include not only the usual properties (mean profiles, surface fluxes, cloud cover and type) but also some not often measured (e.g., flux profiles, mesoscale variability, structure of the inversion). Not all of these properties are easily measured, however, and when coupled with the general difficulties of direct measurements in the PBL (summarized in Chapter Two) this makes a definitive comparison of LES predictions with PBL observations a formidable challenge. Perhaps the innovative use of modern Doppler radars and other new instrumentation will be needed to attain the detailed PBL data necessary for assessing LES predictions.

Due to the difficulty and expense of making measurements in the PBL, the design of PBL experiments has its own formidable challenges. We feel that LES can be useful in this design, particularly in the case of flows (such as those over complex terrain) rich in "large-eddy" phenomena that are difficult to understand or even anticipate a priori. This illustrates what we see as the potentially strong interactive coupling between LES and PBL observations.

Since dispersion experiments in the atmosphere are very difficult and expensive, that aspect of LES performance should be first tested against laboratory measurements, in our opinion. As discussed in Chapter Two, the

Willis-Deardorff measurements of dispersion in a convection tank already stand as a suitable data base for both neutrally and positively buoyant releases.

d. Technology transfer

Because LES models are intricate, computationally demanding, and expensive to use, we do not forsee their availability for routine PBL applications in the near future. Nonetheless, we have identified in Chapter Six several areas where LES studies could almost immediately stimulate technology transfer from PBL research to applications. Thus, we would recommend that an LES development program have an applied component in which LES would be used in

- studying the sources and physics of inherent uncertainty, and quantifying it in dispersion applications;
- developing parameterizations for higher-order-closure models of the PBL;
- developing subgrid-scale parameterizations for larger-scale meteorological models.

7.2 The Management Challenge

This LES program would ideally be carried out, in our opinion, by a group
- with a "critical mass"
- in contact with the small-scale meteorology community
- in contact with the engineering LES community
- with a supercomputer
- with sustained funding
- free to work to high standards.

It is not clear to us that an institution capable of fostering this LES program now exists in this country. While we feel that an Institute for Environmental Fluid Mechanics, perhaps patterned after NCAR, could provide a suitable environment, the realities of today's funding picture make such substantial new starts seem unlikely.

Large sums have been spent on atmospheric dispersion research in this country over the past 20 years, and yet in the perception of some observers the applications of the resulting basic science to practical problems remain disappointing. Some would give high priority to funding realignments which could expeditiously rectify this situation. While our committee does not feel that a "crash" LES program is such an expedient, it does believe that a

carefully designed, well-balanced program having the components we listed could make the next 20 years much more productive.

Our committee feels, therefore, that choosing appropriate roles for LES in the boundary-layer problems of the future, fostering its development for these roles, maintaining an appropriate balance among basic research, development, and applications, all within an austere funding climate, is a formidable management challenge. We will next offer some guidelines, drawn from the experience of the engineering LES and the meteorological communities, on how this challenge could be met.

7.3 Management Guidelines

Our committee feels that certain management strategies could stimulate the LES development we recommend, even with the initial absence of a ready, coherent community. Specifically, we feel that

1. Periodic conferences on turbulent geophysical flows, patterned after the 1980-81 AFOSR-HTTM-Stanford Conference on Complex Turbulent Flows (Kline et al., 1981) could greatly stimulate the growth of an environmental fluid mechanics community.

2. Post-doctoral programs in supercomputer environments, designed specifically for environmental fluid mechanics, could bring talented new workers into the field.

3. Modularization and dissemination of FTS and LES codes and the development of efficient software for managing out-of-core calculations could greatly simplify the task of building LES mdels for PBL applications.

4. Enhancement of laboratory facilities for the simulation of geophysical turbulence could provide some of the data bases needed for the optimum development of LES codes.

5. Our national consciousness about supercomputing is being raised. There is a growing realization that computers can greatly enhance our understanding of the mathematics of nonlinear dynamical processes such as turbulence. Movements are under way at the federal level to facilitate access to supercomputers. This seems a particularly good time for lobbying efforts on the behalf of LES development for environmental fluid mechanics.

6. Substantially enhanced computer graphics software could provide
    supercomputer versions of the flow visualization techniques which
    have traditionally been used in laboratory fluid mechanics. These
    techniques are dramatically displayed in Van Dyke's (1982) An Album
    of Fluid Motion, a collection of photographs of fluid flow which is
    attracting wide attention. Flow visualization is recognized as
    vitally important to fluid mechanics research, and we believe that
    computer graphics will be just as important in the computational
    approach.

7.4 A View of the Future

Supercomputers are not only revolutionizing turbulence research; they are
impacting the entire field of nonlinear dynamics. Describing this impact in
his article, "Computational Synergetics," Zabusky (1984) stresses their use in
what he calls the heuristic mode, in which, he says, computers can "shine the
light of inspiration into areas which had been thought devoid of new concepts
or fundamental truths."

Through a number of striking examples, many from fluid mechanics, Zabusky
convincingly demonstrates the power of computers in mathematics and physics.
Near the end of this article, he looks ahead:

> I believe that computational studies will be as useful in the
> future development of nonlinear science as the accelerators of
> the past were for nuclear and particle science. It is only a
> historical accident that supercomputers became available later
> than the superaccelerators. An important asset of the
> computational physicist or mathematician is the will to use
> the computer resources to the limit when the algorithms are
> working and the physics is puzzling.

The most direct and powerful application of supercomputers to small-scale
meteorology is, in our opinion, large-eddy simulation. Its impacts to date,
while substantial, could be dwarfed by those over the next decade. In order
for that to happen, however, we feel that techniques for manipulating and
displaying LES results will have to be substantially improved. Zabusky
perceives the same need and in his article lucidly describes what he sees as
the necessary attributes of a new generation of facile, interactive graphics
software.

Furthermore, we must expect that many of the exciting advances yet to
come in LES will be made by young researchers, perhaps some not yet out of
school. Zabusky asks:

Are we providing the kind of training in our universities that
our students will need to undertake this style of work at the
nonlinear frontier? I believe not. We will need to find new
methods for teaching students to experiment with computers the
way we now teach them to experiment with lasers or cyclotrons.

Clearly, then, the challenges and opportunities for LES in small-scale
meteorology are, to a large extent, those of supercomputing in physics. An
optimum response will require the participation of a broad group of
individuals and institutions, but will, we believe, bring great rewards.

NUMERICAL SIMULATION OF TURBULENT FLOWS[1]

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1. INTRODUCTION

A century has passed since O. Reynolds demonstrated that fluid flow changes from an orderly and predictable state to a chaotic and unpredictable one when a certain nondimensional parameter exceeds a critical value. The chaotic state, turbulence, is the more common one in most flows at engineering and geophysical scales, and its practical significance, as well as the purely intellectual challenge of the problem, has attracted the attention of some of the best minds in the fields of physics, engineering, and mathematics. Progress toward a rigorous analytic theory has been prevented by the fact that turbulence dynamics is stochastic (often having underlying organized structures) and strongly nonlinear. There are, however, rigorous kinematic results that stem from tensor analysis and the linear constraint of continuity, and these allow a reduction of variables in the statistical description of the velocity field in certain cases, especially for isotropic turbulence. Rigorous dynamical results are available only for limiting cases where the governing equations can be linearized, and although the required limits are seldom approached in practice, the linear analysis provides guidance for model development. In spite of the dearth of rigorous nonlinear results, we have accumulated over the years a surprisingly good qualitative understanding of turbulence and its effects. Indeed, the gems of turbulence lore are the scaling laws for particular domains (either in physical or wave space), which result from the recognition of the

essential variables and the constraint of dimensional invariance. In particular, the Kolmogorov law, and the law of the wall, are so well established that compatability with them is required of any theory or simulation.

All attempts at a statistical theory of turbulence have ultimately been faced with the problem of closure, that is, the specification at some order of a statistical quantity for which no governing equation exists. The success of the closure model depends not only on the flow configuration, but also on the statistical order at which results are desired. When the closure model is inadequate for accurate determination of the desired statistics, the model must be improved, or closure postponed to yet higher order. Most of the closures attempted to date may be classified as either one-point or two-point, depending on the number of spatial points appearing in the desired statistical results. Reviews of the many one-point closures are given by Reynolds (1976) and Lumley (1980). The much more complicated two-point closures [the Direct Interaction Approximation (DIA) and the related Test Field Model (TFM) of Kraichnan (see Leslie 1973), and the Eddy Damped Quasi-Normal Markovian (EDQNM) model of Orszag (1970), Lesieur & Schertzer (1978), and Cambon et al. (1981)] have been limited to homogeneous (usually isotropic) flows, where symmetry allows a reduction of variables.

Progress in the experimental study of turbulence has not been as difficult as that of analysis, but it has required great ingenuity in the collection of data and often in setting up the flows themselves. The results are usually of two kinds: statistical and visual. The velocity statistics are collected by use of hot-wire probes and, more recently, also by use of the laser Doppler velocimeter. Flow visualization has been particularly useful in aiding the interpretation of statistical data and identifying persistent flow structures. The primary difficulty with experimental turbulence data is the lack of it; the theoretician needs a number of statistical quantities, some of which (for example, those involving the pressure) are difficult to measure. A secondary problem is the isolation of the effect of a single parameter; for example, the effect of rotation on the decay of turbulence generated by a screen in a wind tunnel must be separated from the effect of rotation on the turbulence-generation process itself. Modern electronic recording and computing equipment has increased the quantity and quality of available data and has led to more-sophisticated analysis techniques (for example, conditional averages and pattern recognition).

The turbulence problem is so challenging that any research tool found successful in even remotely similar problems is quickly brought to bear. The two-point closures are such examples, as are the concepts of "critical phenomena," "strange attractor," and "renormalization." The high-speed

digital computer is another recently developed tool with obvious application to the problem. The computer is used in other ways in fluid dynamics (see Van Dyke's article in this volume), but its most straightforward use is for "brute force" numerical simulation.

The numerical simulation of turbulence as we know it today rests largely on foundations laid down by the meteorologists at the National Center for Atmospheric Research (NCAR); their early work is reviewed by Fox & Lilly (1972). Since that time, computer capacity has increased by over an order of magnitude as has the number of workers in the field. Although some progress has been made in the efficiency and accuracy of computational algorithms, particularly in the adaptation of spectral methods, the primary pacing item determining our ability to simulate turbulence is the speed and memory size of the computing hardware (Chapman 1979, 1981).

The choice between simulation and experiment for a specific flow reduces to two questions: can the desired data be obtained at the required accuracy, and if so, how much will it cost? At the present time, simulation can provide detailed information only about the large scales of flows in simple geometries, and is advantageous when many flow quantities at a single instant are needed (especially quantities involving pressure) or where the experimental conditions are hard to control or are expensive or hazardous. Simulation cannot provide statistics that require a very large sample or that remain sensitive to Reynolds number even at high Reynolds number. It is particularly advantageous to use both simulation and experiment for delicate questions involving stability or sensitivity to external influences.

Turbulence consists of chaotic motion, and often persistent organized motions as well, at a range of scales that increases rapidly with Reynolds number. This restricts complete numerical resolution to low Reynolds number. When the scale range exceeds that allowed by computer capacity, some scales must be discarded, and the influence of these discarded scales upon the retained scales must be modeled. We shall distinguish between completely resolved and partly resolved simulations by referring to them as "direct" and "large-eddy" (LES), respectively, although these terms are often used interchangeably in the literature to indicate both without distinction. The descriptor "large-eddy" is misleading when the important flow structures to be resolved are extremely small as are those near solid boundaries, and at the dissipation scale at high Reynolds number. The attraction of direct simulation is that it eliminates the need for ad hoc models, and the justification often advanced is that the statistics of the large scales vary little with Reynolds number and can be found at the low Reynolds numbers required for complete numerical resolution. This approach has been successful for unbounded flows where viscosity serves mainly to set the scale of the dissipative eddies, but it has not been successful

for wall-bounded flows, such as the channel flow, where computational capacity has so far not allowed a Reynolds number at which turbulence can be maintained. This is typical of many flows of engineering interest and forces the development of the LES approach.

The basic philosophy of LES is to explicitly compute only the large-scale motions that are directly affected by the boundary conditions and are therefore peculiar to the problem at hand. The small-scale motion is assumed to be more nearly universal, that is, its statistics and their effect upon the large scales can be specified by a small number of parameters. We hope that convergence of the method with increasing resolution will be rapid, because our ability to parameterize the sub-grid scale (SGS) effects should improve as the SGS length and time scales become disparate from those at energetic scales, and also simply because the SGS effects are proportional to the reduced SGS energy. The LES approach lies between the extremes of direct simulation, in which all fluctuations are resolved and no model is required, and the classical approach of O. Reynolds, in which only mean values are calculated and all fluctuations are modeled.

The numerical simulation of turbulence requires judgments with respect to the governing equations, initial and boundary conditions, and numerical resolution and methods. In the following sections we discuss some of the available choices and the results that follow from them.

2. GOVERNING EQUATIONS

We limit our discussion of simulation technique to flows of incompressible Newtonian fluids governed by the Navier-Stokes equations. Effects of buoyancy, compressibility, density stratification, magnetic forces, and passive scalar transport introduce new physical phenomena but increase the simulation difficulty in degree rather than kind. The convective terms of the equations produce a range of scales limited by molecular diffusion, so that with sufficiently low Reynolds number the entire range can be numerically resolved and no modification of the governing equations is required. When computer capacity does not allow complete resolution and the equations are not modified to take this into account, the computed values may have no relation to fluid physics. The numerical algorithm may become unstable as the smallest computed scales accumulate energy or, when energy-conserving numerical approximations are used, the energy may reach a nonphysical equilibrium distribution among the finite degrees of freedom. Orszag (see Fox & Lilly 1972) has demonstrated that energy-conserving numerics in inviscid isotropic flow lead to energy equipartition among the degrees of freedom, and this is often used as a check of algorithms and programming in simulation codes. When the viscosity is not

zero but is too small to allow accurate resolution of the dissipation scales, an energy-conserving algorithm collects energy at the smallest computed scales until the dissipation and cascade rates reach equilibrium. Kwak et al. (1975) show that this excess energy, trapped at the mesh scale rather than cascading to the Kolmogorov scale, produces too rapid an energy transfer from large scales. This would be expected if the small scales act on the large scales as an eddy viscosity with a value, proportional to the length and velocity scales of the trapped energy, that is increased by the entrapment. One of the most important modifications of the Navier-Stokes equations is a mechanism for removal of energy from the computed scales that mimics as closely as possible the physical cascade process. The first step in an LES is then to define the variables that can be resolved and their governing equations.

The values at discrete mesh points of a simulation represent flow variables only in some average sense, and one way to define this sense is to find the differential equations that are exactly equivalent to the discrete approximation of the Navier-Stokes equations (Warming & Hyett 1974). The popular second-order central difference formula for the derivative of a continuous variable, for example, gives exactly the derivative of a second continuous variable that is an average of the first one:

$$\frac{u(x+h)-u(x-h)}{2h} = \frac{d}{dx}\left\{\frac{1}{2h}\int_{x-h}^{x+h} u(\xi)\,d\xi\right\}. \tag{1}$$

This shows how a discrete operator filters out scales less than the mesh size h. The direct use of such operators on the terms of the Navier-Stokes equations then introduces a different averaged variable for each term, depending on the derivative and discrete operator involved. This direct approach is therefore limited to completely resolved flows where the averages cause no information loss and all such averages give the same value. When the Reynolds number is too high for the direct approach, the range of scales can be limited to a resolvable size by explicitly filtering the Navier-Stokes equations. This formally defines the averaging process that separates resolvable from subgrid scales and the SGS stresses that must be modeled. When the smallest scale, $O(\Delta)$, allowed by the filter and the SGS model is sufficiently greater than the smallest scale, $O(h)$, resolved by the mesh, the results of the computation are independent of the choice of numerical algorithm and depend only on the filter and SGS model. Complete separation of physics from numerics is very costly in an LES, where mesh doubling in three directions increases the cost by an order of magnitude or more and in practice $\Delta = O(h)$ in each direction. Thus, resolution of the smallest computed scales is often marginal, and care is required to insure that the truncation error is less than the physical SGS

effects. Leonard (1974) applies the homogeneous filter

$$\bar{f} = \int_{-\infty}^{+\infty} G(\mathbf{x} - \xi) f(\xi) \, d\xi, \qquad f = \bar{f} + f' \tag{2}$$

to the Navier-Stokes equations to obtain the "resolvable-scale" equations

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} \overline{u_i u_j} + \frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} = \nu \nabla^2 \bar{u}_i,$$

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0. \tag{3}$$

Here, and throughout the paper, an overbar denotes a resolvable scale quantity and a prime denotes an SGS quantity. The convective fluxes are

$$\overline{u_i u_j} = \overline{\bar{u}_i \bar{u}_j} + Q_{ij}, \qquad Q_{ij} = \overline{\bar{u}_i u_j'} + \overline{u_i' \bar{u}_j} + \overline{u_i' u_j'}. \tag{4}$$

The equations must be closed by specifying these fluxes as functionals of the resolved variables. The terms containing u' must be modeled, but only the deviation from isotropy has dynamic effect. The $\overline{\bar{u}_i \bar{u}_j}$ term may be computed directly from resolved variables. When the average is uniform over an unbounded homogeneous dimension (space or time) or is a statistical (ensemble) average, the postulates of O. Reynolds lead to $\overline{u_i u_j} = \bar{u}_i \bar{u}_j + \overline{u_i' u_j'}$, but the postulates do not apply to averages over bounded domains (Monin & Yaglom 1971, Leonard 1974). The convolution (2) simplifies to $\bar{f}(k) = G(k) f(k)$ in wave space, from which it follows that $\bar{f}' = G(1 - G) f$ is zero only when G is piecewise constant at values of 0 or 1. Reynolds' average is equivalent to $G(k) = 0$ for $|k| > 0$, and Fourier spectral methods implicitly filter with $G(k) = 0$ for $|k| > k_{max}$. In the latter case $\overline{\bar{u}_i \bar{u}_j} = \bar{u}_i \bar{u}_j$ for resolved k, but $\overline{\bar{u}_i u_j'} \neq 0$ there.

An alternative derivation of the resolvable scale equations by Schumann (1975) averages the equations over the cell volumes of a fixed mesh. This leads directly to the integral form of the Navier-Stokes equations in which time derivatives of cell-volume velocity averages are related to differences of cell-surface average stress and momentum flux. The various surface averages of momentum flux are decomposed as in (4) assuming Reynolds postulates, and the required surface averages of velocity and its gradient are related to volume averages of velocity by Taylor-series expansion. There is an inconsistency between the assumption of piecewise constant velocity required for validity of the Reynolds postulates and the use of Taylor-series expansions, but the resulting equations, except for the SGS model, are precisely those obtained by Deardorff (1970) using the continuous averaging process (1) and second-order numerics on a staggered uniform mesh.

The cell-volume averaging used by Deardorff and Schumann does not satisfy Reynolds postulates, and the difference $\overline{u_i u_j} - \bar{u}_i \bar{u}_j$ is modeled. The part of this, $\overline{\bar{u}_i \bar{u}_j} - \bar{u}_i \bar{u}_j$, that can be computed directly from resolved variables is known as the Leonard term. Leonard (1974) shows that this term removes significant energy from the computed scales and should probably not be lumped with the SGS terms. If direct calculation of the term is difficult he proposes a simple model, based on its Taylor-series expansion:

$$\overline{\bar{u}_i \bar{u}_j} \sim \bar{u}_i \bar{u}_j + \frac{\gamma}{2} \nabla^2 (\bar{u}_i \bar{u}_j) + \cdots, \qquad \gamma = \int_{-\infty}^{+\infty} |\xi|^2 G(\xi) \, d\xi. \tag{5}$$

At low Reynolds number Clark et al. (1979) find this form to be quite accurate when compared with values from a direct simulation. Shaanan et al. (1975) used a numerical operator for the divergence of the flux tensor in the Navier-Stokes equations that has lowest-order truncation error of nearly the form (5), thereby implicitly capturing the Leonard term. Most subsequent authors who explicitly filter the equations simply compute $\overline{\bar{u}_i \bar{u}_j}$ (Mansour et al. 1979). Clark et al. (1977) also find that the measured "cross" terms $C_{ij} = \overline{\bar{u}_i u_j'} + \overline{u_i' \bar{u}_j}$ drain significant energy from the resolved scales. Again, part of the effects can be captured by a Taylor-series expansion of the *resolved scale* velocity:

$$\overline{u_i' \bar{u}_j} \sim \overline{u_i'} \bar{u}_j + \frac{\Delta^2}{12} \frac{\partial \overline{u_i'}}{\partial x_k} \frac{\partial \bar{u}_j}{\partial x_k} + \cdots, \tag{6}$$

where $\overline{u_i'} = \bar{u}_i - \bar{\bar{u}}_i$, and we have used a Gaussian filter, $G(\xi) = \sqrt{(6/\pi\Delta)} e^{-6\xi^2/\Delta^2}$. Clark et al. (1977) propose a different model for the cross terms, but its derivation involves the Taylor-series expansion of the SGS velocity field. The dependence of the modeled terms in (4) upon the filter (for example, the vanishing Leonard term for sharp filters in wave space) suggests that simulation accuracy might be improved by a particular choice. Deardorff (1970) and Schumann (1975) use cell-volume averages related as in (1) to their finite-difference operators, and Chollet & Lesieur (1981) use the sharp filter implied by their Fourier spectral methods. When the choice of filter is divorced from the numerical algorithm, and this can only occur for $\Delta \gg h$, the Gaussian filter (Kwak et al. 1975, Shaanan et al. 1975, Mansour et al. 1978, Moin & Kim 1982) is usually used for homogeneous dimensions because it provides a smooth transition between resolved and subgrid scales and is positive definite (in fact Gaussian) in both physical and wave space. The optimum choice is of course the combination of filter and model that minimizes the total simulation error. The ratio of

filter to mesh resolution, Δ/h, serves primarily to control numerical error, while the form of the filter and the form of the closure model determine the modeling error. The dependence of the model on the filter is studied, in isotropic flow within the TFM framework, by Leslie & Quarini (1979) and, for solutions of the Burgers equation, by Love (1980).

The averaged Navier-Stokes equations (3,4) provide a conceptual framework for the discussion of modeling. The practical value of explicitly filtering the convective terms is a matter of current debate. The Leonard term is $O(\Delta^2)$, so it seems pointless to compute it separately in simulations using second-order numerics with error of $O(h^2)$ unless $\Delta/h \gg 1$ and the filtered field is well resolved. When the Leonard term is not swamped by numerical error, the filter, SGS stresses, and velocity field are related by (4), and the filter and model, $M(u)$, should in principle be selected together to minimize in some sense the modeling error $\overline{u_i u_j} - \overline{\bar{u}_i \bar{u}_j} - M_{ij}(\bar{u})$; the filtered convection $\overline{\bar{u}_i \bar{u}_j}$ is then computed directly. Kwak et al. (1975), for example, assume a Gaussian filter and a Smagorinsky (1963) SGS model and optimize the filter width and model constant by matching decay rate and spectral shape from the LES with experimental data for isotropic turbulence. A general study of filter and model forms has not yet been attempted. But the true filter is always uncertain because of the inherent inability of SGS models to exactly satisfy (4), so that the Leonard term cannot be found without error. An argument against separate treatment of the Leonard term is advanced by Antonopoulos-Domis (1981), who finds that in his LES calculations it moved energy from the small resolved scales to the large ones, rather than to the subgrid scales as predicted by Leonard. Leonard & Patterson (unpublished) point out that in isotropic turbulence the transfer spectrum $T(k)$ associated with the flux $\bar{u}_i \bar{u}_j$ is negative at small k, positive at large k, and is conservative. The transfer spectrum associated with the filtered flux $\overline{\bar{u}_i \bar{u}_j}$ is simply $G(k)T(k)$ and can reasonably be expected to remove energy from the resolved scales. The proper way to determine the effect of the Leonard term is to measure the energy transfer associated with the filtered convective term in an *accurately resolved field*. Studies of this kind by Leonard & Patterson, Clark et al. (1979), and Leslie & Quarini (1979) have verified the energy drain but at a lower magnitude than Leonard's original estimate. Antonopoulos-Domis draws his conclusions from simulations with no viscous or modeled turbulent terms. His results do indicate that the approximate form (5) alone is not sufficient to stabilize the calculation, but they do not indicate the effect of the Leonard term in a well-resolved calculation. A more general problem with explicit filters is the difficulty of extending them to inhomogeneous dimensions, where differentiation and filtering do not in general commute, but this does not seem insurmountable.

The equations of LES are then essentially the original Navier-Stokes equations written for averaged variables, with a filtered convection term and additional terms to model the effects of the unresolved scales. The only change from the original analysis of O. Reynolds is the use of averages over bounded domains, which requires the convective term to be filtered. The crux of the problem remains the closure model.

3. MODELS

Statistical homogeneity in space or time reduces the dimensions of the Reynolds-averaged problem, and all of the effects of fluctuations in the missing dimensions must be accounted for by the model. The variation of correlations in the remaining inhomogeneous dimensions is peculiar to the specific problem and cannot be modeled in a universal way. In an LES the equations are averaged over only small scales and retain all space-time dimensions. The averaging process is chosen to resolve numerically the physical features of interest, and the desired statistics are measured directly from the computed scales. The role of the model is not to provide these statistics directly, but to prevent the omission of the unwanted scales from spoiling the calculation of scales from which statistics are taken.

It is apparent from the LES work to date that the most important contribution of the model is to provide, or at least allow, energy transfer between the resolved and subgrid scales at roughly the correct magnitude. This transfer is usually from resolved to subgrid scales but may be reversed near solid boundaries, where the small productive eddies are not resolved and the SGS model must account for the lost production. Models can be tested either by directly comparing the modeled quantity with the model itself, using data from a reliable source (theory, experiment, or direct simulation), or by using the model in an LES and comparing results with those from a reliable source. The detailed information required for the former test can be supplied only by theory or simulation, and in practice the latter procedure is the more common. This is consistent with the LES philosophy; the model is not required to supply detailed information about the subgrid scales. But there is frequently a need to improve the model's description of physical detail and thus allow increased reliance on the model and lower computation cost. The sequence of model complexity could follow the same path as for the Reynolds-averaged equations, with the introduction of separate equations for the SGS stress or energy (Deardorff 1973). But in an LES the SGS length scales are given by the filter width, and velocity scales can be estimated from the smallest resolved scales. Bardina et al. (1980) suggest that the SGS stresses themselves be modeled by an extrapolation of the computed stresses at the smallest

resolved scales. The simplest model, $\overline{u_i' u_j'} \sim C\overline{u_i'} \, \overline{u_j'} = C(\bar{u}_i - \bar{\bar{u}}_i)(\bar{u}_j - \bar{\bar{u}}_j)$, has been tested by McMillan et al. (1980) using data from direct simulations. The model correlates much better with the data than does a typical eddy-viscosity model, but Bardina et al. find that it is not sufficiently dissipative to stabilize an LES.

The effects of discarded scales on computed ones consist of "local" contributions, which diminish rapidly as the interacting scales are separated, and "nonlocal" contributions, which are significant even for widely separated scales. The interaction between scales of similar size retains the full complexity of the original turbulence problem, so there is little hope of modeling the local effects well. On the other hand, interaction of disparate scales is easier to analyze, so that nonlocal effects can be modeled with greater confidence.

The modern statistical theories of isotropic turbulence (DIA, TFM, EDQNM) provide models in which the roles of the various scales can be determined. Kraichnan (1976) and Leslie & Quarini (1979) evaluate the transfer spectrum within the TFM model, showing explicitly the local and nonlocal (in wave space) effects of the truncated scales on the energy flow within the resolved scales. The transfer spectrum is of the form $T(k) = -2\nu(k)\sqrt{E(k_m)/k_m}\,k^2 E(k) + U(k)$, where k is the wave-number magnitude, k_m is the limit of wave-number resolution, $\nu(k)$ is a nondimensional eddy viscosity, and E is the three-dimensional energy spectrum. The first term arises from stresses like $\overline{\bar{u}_i u_j'}$, while the "backscatter" term $U(k)$ arises from the $\overline{u_i' u_j'}$ stresses. The forms $\nu(k)$ and $U(k)$ depend upon both the filter and the energy spectrum; Kraichnan considers a sharp k filter in an infinite inertial subrange, and Leslie & Quarini extend these results to a Gaussian filter and more-realistic spectra. Kraichnan finds that the local effects are confined to scales within an octave of k_m and are characterized by a rapid rise in transfer as k approaches k_m. The net energy flow across k_m is dominated by this local transfer as described by Tennekes & Lumley (1972). Below this local range, $k < k_m/2$, the viscosity is independent of k [but depends on time through $E(k_m)$], and the backscatter decays like k^4 (Lesieur & Schertzer 1978). This backscatter might be important in unbounded flows, where length scales grow indefinitely and, as Leslie & Quarini note, its form is not well represented by an eddy-diffusion model because neither its magnitude nor anisotropy level are set by the large scales. Their results indicate that a Gaussian filter damps the SGS contribution to the local cascade too severely and broadens its range; this suggests that a sharper filter might be found in which the Leonard term carries the entire local transfer and leaves only the nonlocal effects to be modeled. Chollet & Lesieur (1981) achieve the same end using Kraichnan's effective eddy viscosity to successfully close both EDQNM and LES calculations. Chollet (1982) closes an LES by

coupling it to an EDQNM calculation for the effective eddy viscosity, thus avoiding an assumed SGS energy spectrum. This is a rather elaborate "one-equation" model. The extension of EDQNM to homogeneous anisotropic flows by Cambon et al. (1981) allows application of this approach to less-restricted SGS stresses, but at a great increase in complexity. Yoshizawa (1979, 1982) relates these statistical closures in wave space to the gradient-diffusion closures in physical space by a formal multiscale expansion. The assumption that the SGS time scale, as well as space scales, is disparate from those of the resolved scales leads to SGS stresses that are locally isotropic at lowest order and of gradient-diffusion form (scalar eddy viscosity) at next order. The more interesting limit of commensurate time scales, leading to homogeneous but anisotropic SGS turbulence at lowest order, is prevented by the resulting complexity of the required DIA closure.

The gradient-diffusion model for SGS stresses is usually postulated with appeal to the similar stresses produced by molecular motion. But it is well known (Tennekes & Lumley 1972, Corrsin 1974) that the required scale separation, present in the case of molecular diffusion, does not occur between all of the scales of turbulence. In the Reynolds-averaged equations for flows having a single length and time scale, the gradient-diffusion form is required by dimensional analysis but the model cannot handle multiple scales (Tennekes & Lumley 1972). The eddy-viscosity model of the SGS stress tensor is

$$\tau_{ij} = Q_{ij} - \tfrac{1}{3}Q_{kk}\,\delta_{ij} \sim -2v_T S_{ij}, \tag{7}$$

where v_T is the eddy viscosity, and $S_{ij} = \tfrac{1}{2}(\partial \bar{u}_i/\partial x_j + \partial \bar{u}_j/\partial x_i)$ is the strain-rate tensor of the resolved scales; the SGS energy $\tfrac{1}{3}Q_{kk}$ can be combined with the pressure and has no dynamic effect.

Smagorinsky (1963) proposes an eddy-viscosity coefficient proportional to the local large-scale velocity gradient:

$$v_T = (C_S \Delta)^2 |S|. \tag{8}$$

Here, C_S is a constant, the filter width Δ is the characteristic length scale of the smallest resolved eddies, and $|S| = \sqrt{S_{ij}S_{ij}}$. This model and its variants have been used in numerical simulations with considerable success. Assuming that scales of $O(\Delta)$ are within an inertial subrange so that $|S|$ can be found from Kolmogorov's spectrum, the analysis of Lilly (1966), with a Kolmogorov constant of 1.5, gives values of C_S from 0.17 to 0.21, depending on the numerical approximation for S_{ij}. Subsequent investigators determine C_S in an empirical manner. In large-eddy simulations of decaying isotropic turbulence, Kwak et al. (1975), Shaanan et al. (1975), Ferziger et al. (1977), and Antonopoulos-Domis (1981) obtain C_S by matching the computed energy-decay rate to the experimental data of

Comte-Bellot & Corrsin (1971). For several computational grid volumes and different filters they find C_S to be in the range 0.19–0.24. None of these calculations extends to an inertial subrange, and different treatments of the Leonard stresses and numerical methods are used; thus, the small variation of C_S indicates its insensitivity to the details of the energy-transfer mechanism in isotropic turbulence.

In a simulation of high-Reynolds-number turbulent channel flow, Deardorff (1970) finds that the use of the value of C_S estimated by Lilly causes excessive damping of SGS intensities, but that a value of 0.1 gives energy levels close to those measured by Laufer (1951). Deardorff (1971) attributes this difference in C_S to the presence of mean shear, which is not accounted for in Lilly's analysis. In the calculation of inhomogeneous flows without mean shear, where buoyancy is the primary driving mechanism, Deardorff (1971) finds $C_S = 0.21$ appropriate. Lower values lead to excessive accumulation of energy in one-dimensional energy spectra near the cutoff wave number.

Using flow fields generated by direct numerical simulation of decaying isotropic turbulence at low Reynolds number, Clark et al. (1977, 1979) and McMillan & Ferziger (1979) tested the accuracy of Smagorinsky's model and calculated C_S. They give values of C_S comparable to those obtained empirically in the large-eddy simulations. McMillan et al. (1980), using data from direct simulations of strained homogeneous turbulence, find that C_S decreases with increasing strain rate, which confirms the conclusions of Deardorff (1971). With the mean strain rate removed from the computation of the model, C_S is nearly independent of the mean strain, a highly desirable property for the model. Fox & Lilly (1972) point out that the removal of the mean shear might have allowed Deardorff (1970) to use the higher C_S value of Lilly.

In addition to calculating model parameters, direct simulations are also used to determine how well the forms of the SGS models represent "exact" SGS stresses. For isotropic turbulence, the results show that the stresses predicted by Smagorinsky's model (and other eddy-viscosity models) are poorly correlated with the exact stresses. The model performance is worse still in homogeneous flows with mean strain or shear. The notable success of calculations using the Smagorinsky model seems to reflect the ability of this model to stabilize the calculations, and also shows that low-order statistics of the large scales are rather insensitive, in the flows considered, to the details of the SGS motions.

Several alterations and extensions to Smagorinsky's model have been proposed. A modification consistent with the classical two-point closures replaces the local magnitude of the strain-rate tensor, $|S|$, in (8) with its ensemble average $\langle S \rangle$ (Leslie & Quarini 1979). Although in numerical

solutions of the Burgers equation (Love & Leslie 1979) this modification improves the results, direct testing in isotropic flow by McMillan & Ferziger (1979) shows only a slight improvement. For free-shear flows, Kwak et al. (1975) suggest that it is appropriate to use the magnitude of vorticity $|\omega|$, rather than $|S|$, in (8), because the former vanishes in an irrotational flow. For isotropic turbulence this modification does not cause significant differences in large-scale statistics, but a substantial disparity is reported in small-scale statistics such as the velocity derivative flatness (Ferziger et al. 1977), which indicates the sensitivity of the smallest resolved scales to the SGS model. To account for mean shear in an LES of turbulent channel flow, Schumann (1975) introduces a two-part eddy-viscosity model. One part models the SGS stress fluctuations, and the other part, which reduces to Prandtl's mixing-length model for very coarse grids, accounts explicitly for the contribution of the mean shear.

When the grid resolution near a solid boundary is inadequate, the SGS flow field includes highly dynamic anisotropic eddies that contribute a significant portion of the total turbulence production and do not take a passive and dissipative role. Moin & Kim (1982), like Schumann, use a two-part eddy-viscosity model to account fully for the contributions to energy production by the finely spaced high- and low-speed streaks near the wall (see Section 4 and Kline et al. 1967) that are not adequately resolved in the spanwise direction:

$$\tau_{ij} = -v_T(S_{ij} - \langle S_{ij} \rangle) - v_T^{\pm}(y)\langle S_{ij} \rangle. \tag{9}$$

Here $\langle \; \rangle$ indicates an average over planes parallel to the walls. The first term in (9), the Smagorinsky model with mean shear removed, has essentially dissipative and diffusive effects on the resolvable scale turbulence intensities, $\sqrt{\langle(\bar{u}_i - \langle \bar{u}_i \rangle)^2\rangle}$. The second term accounts for the SGS energy production corresponding to SGS dissipation of mean kinetic energy $\langle \bar{u} \rangle^2$ but, in contrast to the first term, does not contribute to the dissipation of resolvable-scale turbulent kinetic energy. It does, however, indirectly enhance resolvable-scale energy production by representing the effect of the SGS stresses on the mean-velocity profile. Indeed, when Moin & Kim (1982) excluded the second term of (9) the computed flow did not transfer sufficient mean energy to the turbulence to sustain it against *molecular* dissipation. The characteristic length scale associated with $v_T^{\pm}$ is Δ_3, the filter width in the spanwise direction (normal to the mean flow and parallel to the wall), multiplied by an appropriate wall-damping factor to account for the expected y^3 or y^4 behavior of the Reynolds shear stress near the wall ($y = 0$). The influence of $v_T^{\pm}$ diminishes as the resolution of the spanwise direction is increased and the wall-layer streaks are better resolved.

Eddy-viscosity models of the type described above implicitly assume that

the SGS turbulence is in equilibrium with the large eddies and adjusts itself instantaneously to changes of the large-scale velocity gradients. It may be desirable (certainly in transitional flows) to allow a response time for the SGS eddies to adjust to the changes in the resolvable flow field. Following Prandtl, Lilly (1966) assumes an eddy viscosity proportional to the SGS kinetic energy q^2, i.e. $v_T = c\Delta q$. The equation for q^2, derived formally from the Navier-Stokes equations, contains several terms that must be modeled. Schumann (1975) successfully uses this model for the fluctuating SGS stresses in his calculation of turbulent flows in channels and annuli. Grotzbach & Schumann (1979) extend the model to lower Reynolds numbers. In addition to dividing the SGS stresses into mean and fluctuating parts, a noteworthy feature of Schumann's formulation is its explicit allowance for anisotropic grids. Different characteristic length scales and dimensionless coefficients determined by grid geometry appear in the representation of the various surface-averaged SGS stresses. The utility of the model is demonstrated by its ability to simulate turbulent flow in an annulus, with relatively high grid anisotropy, by changing only the mesh-geometry parameters. Parameters of a physical nature retained the values used in the channel flow calculations (Schumann 1975).

Deardorff (see Fox & Deardorff 1972) finds that the Smagorinsky model smears out the mean temperature gradient that occurs when buoyant convection is terminated by a stably stratified overlayer. For a more realistic model, Deardorff (1973) resorts to transport equations for the SGS stresses. This involves 10 additional partial differential equations. The closure models in these equations are essentially analogous to the corresponding models in the Reynolds-averaged equations. These models may not be appropriate because the behavior and relative importance of the various correlations involving only small scales are different than those involving the total turbulence (Ferziger 1982). Although the transport model does lead to improved results, the prospect of such a complex treatment of the SGS stresses is less attractive to us than a judicious distribution of mesh points and the possibility of extracting more-accurate models directly from information carried at the resolved scales.

In the discussion of the equations and models for LES we have considered flows in which the statistics of interest are determined by the large scales. This is appropriate for engineering purposes, but there are also very fundamental and interesting questions about the small scales to be answered. These are concerned with intermittency and structure at small scale, and the implications for Kolmogorov's universal equilibrium hypothesis and its later modifications. Siggia (1981) outlines a conceptual procedure analogous to LES in which the large scales are modeled and the small scales are computed. The model for the missing large scales appears as

a forcing term in the equations for the small scales. Siggia argues that if the large-scale effects depend on a small number of parameters (the dissipation rate is an obvious one) and the model is accurate enough, the limited scale range of the simulation might represent the intermittency achieved by the larger range of scales occurring at high Reynolds numbers. Unfortunately this is not possible in a calculation based on a periodic field in a fixed mesh, because the small-scale spatial intermittency that can be represented is directly limited by the number of mesh points and this geometric constraint cannot be modeled away. The vortex method of Leonard (1980) is not grid limited and is a more natural way to describe the intermittent vorticity fields occurring at high Reynolds numbers.

4. RESOLUTION REQUIREMENTS

Over two decades ago Corrsin (1961) demonstrated that the direct numerical simulation of high-Reynolds-number flows places an overwhelming demand on computer memory and speed. [See Chapman (1979) for a comprehensive study of the grid requirements for computational aerodynamics.] In direct simulations the number of spatial grid points is determined by two constraints: first, the size of the computational domain must be large enough to accommodate the largest turbulence scales (or the scale of the apparatus), and second, the grid spacing must be sufficiently fine to resolve the dissipation length scale, which is on the order of the Kolmogorov scale, $\eta = (v^3/\varepsilon)^{1/4}$. The ratio of these two scales (cubed) provides an estimate for the total number, N, of mesh points. In turbulent channel flow, for example, macroscales in the directions parallel to the walls determined from the two-point correlation measurements of Comte-Bellot (1963) and the average dissipation rate $\varepsilon = u_\tau^2 U_m/\delta$ give $N \simeq (6\mathrm{Re}_m)^{9/4}$ (Moin 1982); here Re_m is the Reynolds number based on the channel half-width, δ, and the average flow speed, U_m; and $u_\tau = \sqrt{\tau_w/\rho}$ is the wall shear velocity determined by the shear stress at the wall, τ_w, and the fluid density ρ. It is assumed that four grid points in each direction are required to resolve an eddy, and that $U_m/u_\tau \simeq 20$. Temporal resolution of the smallest computed eddies requires the time step Δt to be on the order of $(v/\varepsilon)^{1/2} = (\delta/u_\tau)\,\mathrm{Re}_m^{-1/2}$. At the moderate Reynolds number $\mathrm{Re}_m \approx 10^4$, roughly 5×10^{10} grid points and 2×10^3 time steps are necessary for the flow to reach a statistically steady state (a total flow time of $100\delta/U_m$). Such a computation is beyond the capabilities of presently available computers. However, if the bulk of the dissipation occurs at scales larger than 10η rather than η, direct simulation of channel or pipe flow may be possible in the near future at the lowest Reynolds numbers studied experimentally ($\mathrm{Re}_m \sim 2500$; see Eckelmann 1974).

In contrast to wall-bounded turbulent shear flows, which cannot be sustained below a critical Reynolds number, homogeneous and free-shear flows remain turbulent at Reynolds numbers for which all scales of motion can be resolved. The large-scale features of these flows are nearly independent of Reynolds number, and statistics determined from them are relevant at higher Reynolds numbers. However, in the simulation of unbounded shear flows such as turbulent jets and mixing layers (especially at low Reynolds numbers), the computational domain must be large enough to allow development of the long wavelength instability typical of these flows.

In LES the resolution requirements are determined directly by the range of scales contributing to the desired statistics and indirectly by the accuracy of the model. The less accurate the model, the further the modeled scales must be separated from the scales of interest. In engineering calculations the important scales contain the dynamic physical events responsible for turbulent transport of heat and matter and the production of turbulent energy. Near walls the principal flow structures are high- and low-speed streaks, which are finely spaced in the spanwise direction (Kline et al. 1967) and provide most of the turbulence energy production. The mean spanwise spacing of the streaks is about 100 wall units ($100v/u_\tau$), but streaks as narrow as 20 wall units probably occur and would require $h_3^+ \sim 5$ for complete spanwise resolution (Moin 1982). Similar considerations in the streamwise direction lead to $h_1^+ = 20$ to 30. Using 64 grid points normal to the wall (with nonuniform spacing to resolve the viscous sublayer and outer layers) and with computational periods in directions parallel to the walls chosen in accordance with two-point correlation measurements, the total number of grid points is estimated to be $N \sim 0.06\ \text{Re}_m^2$. Although at high Reynolds numbers this is prohibitively large, detailed simulation of the important large eddies can be performed at low Reynolds numbers ($\text{Re}_m \sim 5000$) with presently available computers. The Reynolds number of resolvable flows can be significantly increased when a fine mesh in the lateral directions is embedded near the walls (Chapman 1979), but for practical applications much computer power is still needed to calculate the flow in this extremely thin layer. If the wall-layer dynamics can be replaced by reliable outer-flow boundary conditions (see Section 5.2), the number of grid points becomes low enough to use LES for engineering computations on current computers (Chapman 1981).

Another practical difficulty in both direct and large-eddy simulations is the cost of obtaining an adequate sample for the flow statistics. The various scales of motion are not equally sampled; the scale sample is inversely proportional to the scale volume. With appeal to the ergodic hypothesis, ensemble averages can be replaced by averages over homogeneous space-

time dimensions. For low-order velocity statistics a sample of 10^3 nodes appears adequate, but much larger samples are required for statistics of intermittent velocity derivatives and this problem increases with Reynolds number (Fox & Lilly 1972, Ferziger et al. 1977, Siggia 1981). When the homogeneous dimensions (there is usually at least one) do not provide an adequate sample, the statistics can be collected from an ensemble of flows evolving from independent initial conditions, but this is very costly and poses a serious problem for simulation of inhomogeneous flows.

5. NUMERICAL METHODS

Numerical implementation of the governing equations consists of four main issues: numerical approximation of spatial derivatives, initial and boundary conditions, time-advancement algorithm, and computer implementation and organization. In each category there are options available, and the choice of the overall algorithm depends on the problem under consideration, the cost, and the computer architecture.

5.1 *Spatial Representation*

Second- and fourth-order finite differences and spectral methods are used to approximate spatial derivatives. Since turbulent flows involve strong interaction among various scales of motion, special care should be taken that numerical representation of derivatives be faithful to the governing equations and the underlying physical mechanisms. For example, approximations with appreciable artificial viscosity, such as upwind difference schemes, significantly lower the effective Reynolds number of the calculation, and their dissipative mechanism distorts the physical representation and dynamics of large as well as small eddies. The formal order of accuracy associated with a difference method, which defines the asymptotic error for infinite resolution, may be less important than the accuracy of the method at the coarse resolution applied at the smallest computed scales. The accuracy of a method at various scales is illustrated by its ability to approximate the derivative of a single Fourier mode e^{ikx} (Mansour et al. 1979). For a given number of grid points, all difference schemes are inaccurate for values of wave number k near π/h, the highest wave number that can be represented on the grid. However, for intermediate values of k some schemes are significantly more accurate than others having the same formal order of accuracy.

The spectral method (Gottlieb & Orszag 1977) is a very accurate numerical differentiator at high k values. In this method the flow variables are represented by a weighted sum of eigenfunctions, with weights determined using the orthogonality properties of the eigenfunctions. The

derivatives are obtained from term-by-term differentiation of the series or by using the appropriate recursion relationships (Fox & Parker 1968). The choice of eigenfunctions depends on the problem and the boundary geometry and conditions. For problems with periodic boundary conditions Fourier series are the natural choice, but for arbitrary boundary conditions orthogonal polynomials that are related to the eigenfunctions of singular Sturm-Liouville problems should be used (Gottlieb & Orszag 1977). Expansions based on these polynomials do not impose parasitic boundary conditions on higher derivatives, and for smooth functions they provide rapid convergence independent of the boundary conditions.

The difference between spectral and "pseudo-spectral" approximations is in the way products are computed (Orszag 1972). The advantage of the more expensive spectral method is the exact removal of aliasing errors (Orszag 1972); Patterson & Orszag (1971) give efficient techniques for handling aliasing errors arising in bilinear products. These errors are not peculiar to pseudo-spectral methods; finite-difference approximations of products also contain aliasing errors, but the errors are less severe owing to the damping at high k of the difference approximations. Aliasing errors usually increase with the order of accuracy of difference schemes (Orszag 1971).

One serious consequence of aliasing errors is the violation of the invariance properties of the Navier-Stokes equations. It is easily shown that in the absence of viscous terms and time-differencing errors, the governing equations conserve mass, momentum, energy, and circulation. Aliasing errors can violate these invariance properties and lead to nonlinear numerical instabilities (Phillips 1959). Lilly (1964) demonstrates that the staggered-mesh difference scheme (see Harlow & Welch 1965) preserves these invariance properties. When the nonlinear terms in the momentum equations are cast in the rotational form, $\omega \times u + \nabla(u^2/2)$, properly invariant numerical solutions are obtained with pseudo-spectral and most finite-difference methods (Mansour et al. 1979).

For sufficiently smooth functions, spectral methods are more accurate than difference schemes having the same number of nodes. In contrast to higher-order difference methods, which require special treatment near the boundaries, spectral methods allow proper imposition of the boundary conditions. However, for the flow field to be sufficiently smooth, the smallest scale of motion present should be well resolved on the computational grid; otherwise, the rapid convergence of spectral methods is badly degraded. Cost constraints usually prohibit thorough resolution of the small scales; in direct simulations this means a mesh too coarse to capture the dissipation scales and in LES calculations means a filter or SGS model that does not remove sufficient energy from the small scales. In simulations

of "two-dimensional turbulence" in a periodic box, Herring et al. (1974) find that the accuracy of spectral calculations is comparable to that of second-order (conservative but aliased) difference calculations having approximately twice the number of grid points in each direction. The advantage of the spectral method as an accurate differentiator is limited by the error that arises from truncation of small scales produced by the nonlinear terms.

A very important attribute of spectral methods is their self-diagnosis property. Inadequate grid resolution is reflected in excessive values of high-order expansion coefficients (Herring et al. 1974, Moin 1982). Fourier analysis of finite-difference solutions can also reveal poor resolution (Grotzbach 1981), but damping at high wave numbers masks its detection until the computational grid is insufficient to represent even the larger scales of motion.

5.2 *Boundary and Initial Conditions*

In turbulence simulations, the major difficulty with specification of boundary conditions occurs at open boundaries where the flow is turbulent. The flow variables at these boundaries depend on the unknown flow outside the domain. The unavoidably ad hoc conditions specified at these boundaries should be designed to minimize the propagation of boundary errors. Periodic boundary conditions are generally used for directions in which the flow is statistically homogeneous, but this implies that quantities at opposite faces of the computational box are perfectly correlated. If the periodic solution obtained is to represent turbulence, the period must be significantly greater than the separation at which two-point correlations vanish. The computed two-point correlation functions then serve as a good check of the adequacy of the size of the period.

Periodic boundary conditions for homogeneous turbulence subjected to uniform deformation may be applied only in a coordinate system moving with the (linear) mean flow. In this system the mean convection relative to the mesh vanishes, and the equations do not refer explicitly to the space variables. However, the computational grid is being continuously deformed, and the calculations must be stopped when the domain becomes so distorted that the flow cannot be resolved in all directions (Roy 1982). In the case of uniform shear, a convenient remeshing procedure (Rogallo 1981, Shirani et al. 1981) allows the computations to continue until the scale of the largest resolved eddies becomes bounded by the period. A clever implementation of the procedure for a finite-difference calculation by Baron (1982) uses shifting boundary values on a fixed mesh. The problem of length-scale growth is common to both experiments and computations. In homogeneous flows or unbounded inhomogeneous flows, the macroscales of turbulence grow until they reach the dimensions of the wind tunnel or the

size of the computational box. When this occurs, meaningful statistics cannot be obtained from the large scales. To study the evolution of the flow for longer times it is tempting to use a coordinate transformation that continuously expands the computational box in time, but such a transformation reintroduces explicit spatial dependence in the governing equations. On the other hand, the calculation can be interrupted and the mesh rescaled to cover a new range of larger scales. The interpolation of the existing field to the new mesh causes some information loss; to minimize the damage the process should be carried out while the two-point correlations still show a significant uncorrelated range.

One of the more challenging, and virtually untouched, problems is that of turbulent inflow and outflow boundary conditions in nonhomogeneous directions. The inflow problem appears to be more troublesome, since in most cases the influence of the upstream conditions persists for large distances downstream. Of course, one way to avoid the problem is to prescribe a small orderly perturbation on an incoming laminar flow and follow the flow through transition to turbulence. However, in addition to more stringent requirements on the treatment of the small-scale motions in transitional flows, the required length of the computational box for the *entire process is prohibitively large in some cases. The use of* turbulent inflow and outflow conditions appears to be a practical necessity for flows such as boundary layers, where linear-stability theory predicts a long transitional zone.

The implementation of inflow and outflow conditions in simulations of free turbulent shear flows has so far been avoided by use of the "frozen turbulence" approximation. The physical problem, which is homogeneous in time but not in the mean-flow direction, is replaced by a computational problem that is homogeneous in the flow direction but not in time. The inflow condition is replaced by an initial condition, and periodic boundary conditions in the mean-flow direction are applied. Although the time-developing approximation of the "real flow" has most of its features, important differences remain. In a spatially developing turbulent mixing layer, for example, the mean streamlines within the layer are inclined to the direction of the flow outside the layer, but those in the time-developing flow are not.

Two approaches have been taken for implementing irrotational free-stream conditions in free-shear flows. Orszag & Pao (1974), Mansour et al. (1978), and Riley & Metcalfe (1980a) use a finite computational domain with stress-free boundary conditions in which the normal velocity and the normal derivative of the tangential velocities are zero. The turbulence field is confined to the central region of the domain and is surrounded by irrotational flow that extends to the boundaries. The subsequent use of

Fourier series implies the existence of image flows above and below the computational box that influence the dynamics of the flow inside. A better approach (Cain et al. 1981) maps the infinite domain into a finite computational box and applies the free-stream (or no-stress) boundary conditions at the boundaries of the transformed domain. The coordinate transformation used by Cain et al. allows a fairly simple use of Fourier spectral methods.

The specification of boundary conditions at smooth solid boundaries does not pose any difficulty; the velocity at the wall is the wall velocity. In the vicinity of the wall, the flow field is composed of small, energetic eddies associated with large mean-velocity gradients (see Section 4). For practical applications it is desirable to avoid the high cost of resolving this wall region by replacing flow near the wall with boundary conditions applied somewhat away from the wall. In simulations of high-Reynolds-number turbulent channel flow, Deardorff (1970) and later Schumann (1975) modeled the flow near the wall by applying such boundary conditions in the logarithmic layer. Once again it is not clear how to specify boundary conditions within a turbulent flow. For example, Schumann (1975) assumes that the fluctuations of wall shear stress, τ_w, are perfectly correlated with those of the streamwise velocity one mesh cell from the wall. Space-time correlation and joint probability density measurements of τ_w and u by Rajagopalan & Antonia (1979) support this assumption very close to the wall provided that a (sizable) time delay between these two quantities is introduced (see also Eckelmann 1974). The accuracy of this assumption degrades as the point of application of boundary conditions moves away from the wall; the normalized correlation is unity at the wall but is only about 0.5 in the logarithmic layer at $y^+ = 40$ ($y/\delta = 0.031$) (Rajagopalan & Antonia 1979). However, Robinson (1982) reports a correlation as high as 0.7 at $y^+ = 300$ ($y/\delta = 0.03$) in experiments at an order of magnitude higher Reynolds number ($Re_\theta = 32,800$). These experimental results indicate that the u-τ_w correlation at a fixed y^+ improves with increasing Reynolds number, but at least part of this apparent improvement results from inadequate probe resolution at high Reynolds numbers. Robinson's wire length extends 200 wall units in the spanwise direction. Nevertheless, Schumann's assumption of u-τ_w correlation is reasonable and can be improved by including a space-time shift. Chapman & Kuhn (1981) propose a two-dimensional wall-layer structure retaining only the transverse spatial variation. They use detailed experimental data to set the length scales and phase relations of the velocity at the outer edge of the layer and obtain good agreement with experiment for the internal layer structure. Their wall-layer edge conditions have not yet been used as boundary conditions for the outer flow. The detailed pressure-velocity data provided

by simulation (Moin & Kim 1982, Kim 1983) should be useful for the formulation of wall-layer edge conditions of the kind proposed by Chapman & Kuhn.

A three-dimensional velocity field satisfying the continuity equation and boundary conditions must be specified to initialize the calculation. Within these constraints, a random fluctuating velocity field is superimposed on a prescribed mean-velocity profile. Although the initial turbulence field can be defined with the desired intensity profiles and energy spectra, its higher-order statistics become physically realistic only after an adjustment period (see Orszag & Patterson 1972, Riley & Metcalfe 1980a). For example, the velocity derivative skewness is initially zero but quickly rises to a realistic value. The evolution of time-developing flows (those that never reach a statistically steady state) is often quite sensitive to the initial conditions for the large scales.

5.3 *Time Advancement*

Starting from initial conditions, the governing equations are advanced in time subject to the incompressibility constraint. We discuss time-advancing algorithms as they are applied to the incompressible Navier-Stokes equations. The additional SGS terms in the LES equations pose little additional numerical difficulty, and virtually identical numerical methods are used.

Time advancement may be done either explicitly or implicitly; explicit schemes are much easier to implement and have a much lower cost per step. The popular second-order explicit Adams Bashforth and Leapfrog schemes require only one evaluation of the time derivatives per step, but they do require retention of variables at step $n - 1$ in order to advance from step n to $n + 1$. The self-starting Runge-Kutta schemes (second, third, and fourth order) cost more per step but have better stability properties and therefore allow larger steps. The multiple evaluations of nonlinear terms required by Runge-Kutta methods can be used to reduce the cost of controlling aliasing errors in Fourier spectral calculations (Rogallo 1981).

When using explicit methods, the incompressibility constraint at each time step is usually enforced by solving a Poisson equation for pressure rather than by direct use of the continuity equation. To satisfy the discrete continuity constraint, the discrete Poisson problem must be derived using the same differencing operators used in the discrete momentum and continuity equations (Kwak et al. 1975). The staggered-grid difference scheme (see Harlow & Welch 1965) leads to a particularly simple Laplacian operator, whereas with standard centered-difference methods the operator is less compact and causes spatial pressure oscillations due to the uncoupling of even and odd points.

The choice of proper boundary conditions for the pressure equation is ambiguous (Moin & Kim 1980). Usually the Neumann boundary condition obtained from the normal momentum equation is used, but a Dirichlet boundary condition can also be derived from the tangential momentum equations. When spectral methods are used with explicit time advancement, the fact that both conditions cannot be simultaneously enforced implies the inability to impose complete velocity boundary conditions (Moin & Kim 1980). With the second-order staggered finite-difference scheme, the need for pressure boundary conditions does not arise. The continuity equation at the interior cells, together with the momentum equations (at the interior grid points) and the velocity boundary conditions, leads to a closed system of algebraic equations for pressure.

The root of this difficulty with spectral methods is that explicit methods treat the governing equations as an initial-value problem rather than as a boundary-value problem. Implicit methods require the solution of a boundary-value problem at each time step, thus allowing the natural imposition of velocity boundary conditions. Moreover, in simulations of wall-bounded flows, implicit treatment of the viscous terms overcomes the severe restriction on time step that arises from the small grid spacing normal to the wall. For these reasons all the calculations that extend to the wall use semi-implicit time-advancement algorithms (Orszag & Kells 1980, Moin & Kim 1980, 1982, Kleiser & Schumann 1979). In these calculations the nonlinear terms are advanced by the Adams Bashforth method. Fourier expansions are used in homogeneous dimensions, and either Chebyshev polynomial expansions or second-order difference methods are used in the direction normal to the wall. Recently, Leonard & Wray (1982) have developed a semi-implicit spectral method based on expansion in divergence-free vector functions. In this representation of the velocity, each term satisfies the continuity equation as well as the boundary conditions. Since the continuity constraint is satisfied by the expansion functions, pressure does not appear and only two velocity components are required to define the velocity field; this significantly reduces computer memory requirements. In wall-bounded flows the time step required for accurate resolution (see Section 4) is much larger than that required for convective stability, which suggests that advancement of the convective terms by implicit methods may be advantageous. Deardorff (1970) and Schumann (1975) translate the coordinate system at constant speed, reducing the mean convection velocity relative to the mesh to allow increased time steps. Alternatively, convection by the mean velocity can be handled implicitly; this is much simpler than a complete implicit treatment.

For problems in general geometries the computational complexity of spectral algorithms is not appreciably greater than that of difference

algorithms when the boundary conditions allow use of explicit time advancement and the physical domain can be analytically mapped to a simple computational domain. But the linear convective stability criterion for the explicit advancement is more severe (by a factor of π for second-order central differences). With fully or partially implicit time advancement the computational complexity of spectral algorithms is much greater than that of difference algorithms. The nonconstant coefficients that arise when a complicated physical domain is mapped to a simple computational domain lead to dense matrix equations for the spectral coefficients. It is impractical to solve these equations by direct techniques; only iterative procedures appear to be feasible (Orszag 1980), and the accuracy and efficiency of the method depend on the number of iterations required to obtain the converged solution at the next step.

6. RESULTS

The flows simulated to date fall into one of three classes: homogeneous (unbounded), unbounded inhomogeneous, and wall bounded. The emphasis of the work can be classified as fundamental physics, development of simulation technique, and application to real problems. In the preceding sections we have discussed some of the work on technique. In this section we present typical fundamental results for three simple shear flows: homogeneous turbulence in uniform shear, the evolution of a turbulent mixing layer, and turbulent channel flow. These flows exhibit many of the complications found in real engineering problems. The homogeneous shear flow introduces anisotropy and production at large scales, the mixing layer adds turbulent diffusion and intermittence at the large scales, and the channel introduces solid boundaries near which all of these complications occur at small scales as well. These three flows are well documented by high-quality experimental data and have been simulated using a variety of numerical methods and a range of resolution.

Turbulence in uniform shear exhibits growing length scales, $O(L)$, and velocity scales, $O(q)$, which appear to approach fixed ratios as the flow evolves (Harris et al. 1977), and the characteristic time of the turbulence, $O(L/q)$, locks on to the characteristic time of the shear, $O(S^{-1})$. It is plausible that the turbulence ultimately attains a self-similar structure with exponential growth of length and velocity scales (Rogallo 1981). The early evolution of isotropic turbulence subjected to uniform shear is predicted well by the linear theory of rapid distortion (Deissler 1961, 1972). Although this theory incorrectly predicts ultimate turbulence decay, its prediction of the Reynolds-stress anisotropy and two-point correlations is surprisingly accurate (Townsend 1976). The first simulation of homogeneous shear was
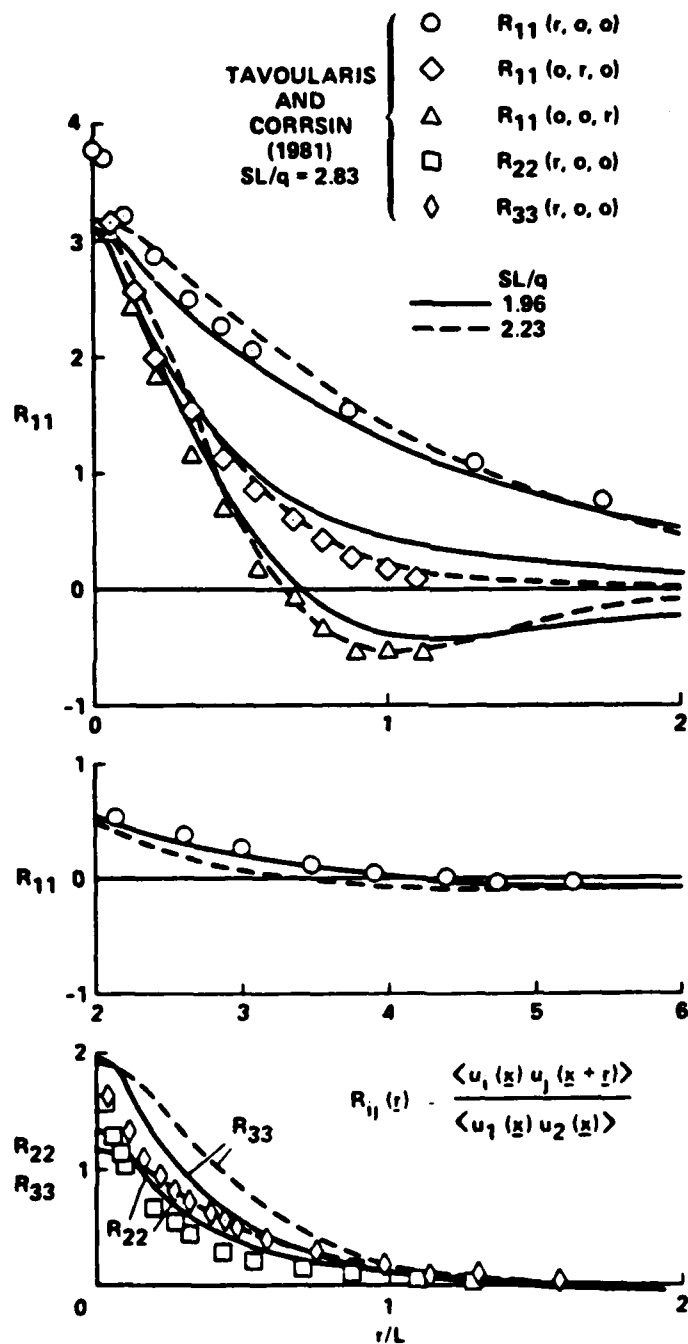
Figure 1 Self-similarity of the autocorrelations in homogeneous shear turbulence (from Rogallo 1981).

the 16 × 16 × 16 finite-difference LES by Shaanan et al. (1975). Their results agree qualitatively with the experimental data, even though periodic boundary conditions were applied on a fixed mesh (see Section 5). More details of the flow are obtained in the 64 × 64 × 64 direct spectral simulations of Feiereisen et al. (1981) and Shirani et al. (1981) in which compressibility effects and passive scalar transport, respectively, are studied. The results of Rogallo's (1981) 128 × 128 × 128 direct spectral simulation indicate that even at a macroscale Reynolds number an order of magnitude below that of Tavoularis & Corrsin (1981), the large-scale statistics of the experiment can be reproduced. A major difficulty is the definition of a characteristic length for the energy-containing scales. The integral scale depends strongly on the largest computed scales for which the statistical sample is poor. In Figure 1 the computed correlations for two simulations are compared with the data of Tavoularis & Corrsin. The correlations are normalized by the turbulent shear stress rather than normal stresses, and the separation is made nondimensional by reference to the longitudinal integral scale in the mean-flow direction. This scaling should collapse the correlations of the large scales; the correlations of streamwise velocity collapse well for the different Reynolds numbers and characteristic times ratios, SL/q, but collapse for the transverse velocity components is less satisfying.

The calculated flow fields can be used as detailed data for the development and testing of closure models. As an example, the tensor sum of the pressure-strain correlation (the "slow" term) and the deviator of dissipation,

$$\varepsilon\phi_{ij} = -2\overline{pS_{ij}} + 2(\varepsilon_{ij} - \tfrac{1}{3}\varepsilon\,\delta_{ij}), \qquad \varepsilon_{ij} = \nu\overline{\frac{\partial u_i}{\partial x_k}\frac{\partial u_j}{\partial x_k}}, \quad \varepsilon = \varepsilon_{ii} \qquad (10)$$

is usually modeled in a Reynolds-stress closure (Lumley 1980) by a scalar multiple of the Reynolds-stress anisotropy tensor, $\phi_{ij} \sim \beta b_{ij}$, where $b_{ij} = \overline{u_i u_j}/\overline{u_k u_k} - \tfrac{1}{3}\delta_{ij}$.

Lumley proposes that the scalar coefficient depends on Reynolds number, the invariants of the stress tensor, and other relevant scalars of the flow. The two tensors (Figure 2a) are indeed correlated in the calculated fields, and the collapse obtained by the linear model (Figure 2b) supports its use (but its performance in other anisotropic homogeneous flows does not :

Figure 2 Lumley's (1980) linear model of pressure-strain correlation and dissipation anisotropy. (a) Dependence of modeled tensor on Reynolds-stress anisotropy tensor; (b) comparison of modeled and measured values; (c) variation of model coefficient with Reynolds number. The data points represent independent flow fields at a wide range of parameters (from Rogallo 1981).
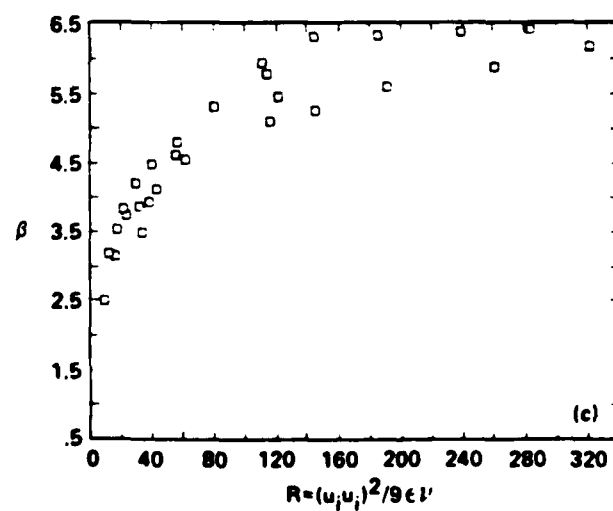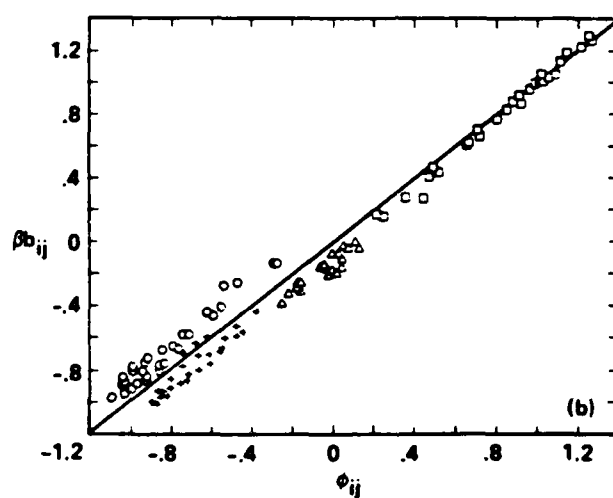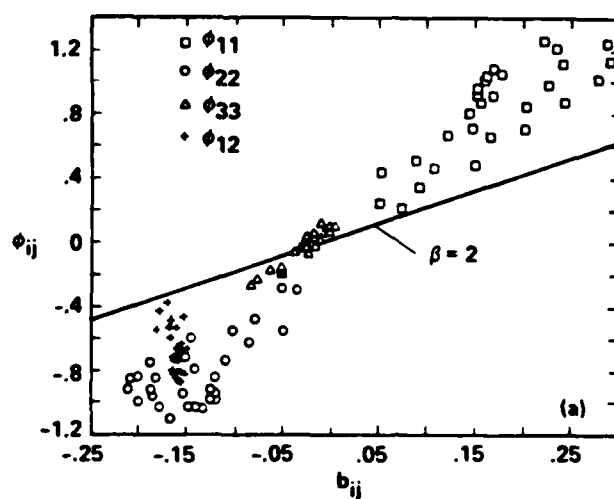
see Rogallo 1981). The orderly nature of the small remaining error suggests the possibility of higher-order model terms. The increase of the model coefficient, β, with Reynolds number (Figure 2c) has been predicted by Lumley, but it should be noted that other scalar attributes of the flow, particularly the ratio of shear and turbulence time scales, are important and they are also varying among the data shown.

The mixing layer separating two uniform streams of differing speed has been studied analytically, experimentally, and recently by simulation. Much of the recent work is concerned with the observed organized vortical structures that result from Kelvin-Helmholtz instability in turbulent layers and their downstream growth by pairing (Roshko 1976). It is found experimentally that the evolution of the layer is strongly influenced by imposed perturbations, and the simulations indicate an analogous sensitivity to initial conditions. Simulations of the LES type have been performed at low resolution by Mansour et al. (1978) and Cain et al. (1981). In the calculations of Mansour et al., the roll-up stage of the flow is inhibited by a mesh domain too short to support unstable waves. When vortex cores are included in the initial field the eddy-viscosity model, in the presence of the mean shear, prevents the proper growth of energy and length scales. The problem appears to be simply one of inadequate resolution. The mesh of Cain et al., on the other hand, is scaled to include the fundamental instability wave and its subharmonic. Roll up of the layer occurs, with the resulting vortices meandering in the spanwise direction and pairing locally to form a network of vortex tubes. Riley & Metcalfe (1980b), using a $32 \times 32 \times 32$ direct spectral simulation, show (as do Cain et al.) that the presence of an energetic two-dimensional instability wave modulates the layer growth; the early growth is more rapid, but once roll up has occurred growth is delayed until the vortices approach each other (by turbulent diffusion, convection by a subharmonic, spanwise variations in proximity, etc.) closely enough for pairing to occur. The spanwise vorticity field of a turbulent mixing layer (Figure 3a) clearly shows coherent structures, even though the layer growth is statistically self-similar. The structures are not simple two-dimensional vortices however, as the vorticity at another spanwise plane (Figure 3b) indicates. Metcalfe & Riley (1981) increase the computational domain to capture the subharmonic of the instability wave. These $64 \times 64 \times 64$ mesh results confirm their earlier results, and the larger domain eliminates a spurious growth of turbulence intensity found there. This flow illustrates the importance of not constraining potentially important scales, in this case the instability scale.

The most extensive application of LES has been the calculation of fully developed turbulent channel flow. In the first realistic numerical simulation
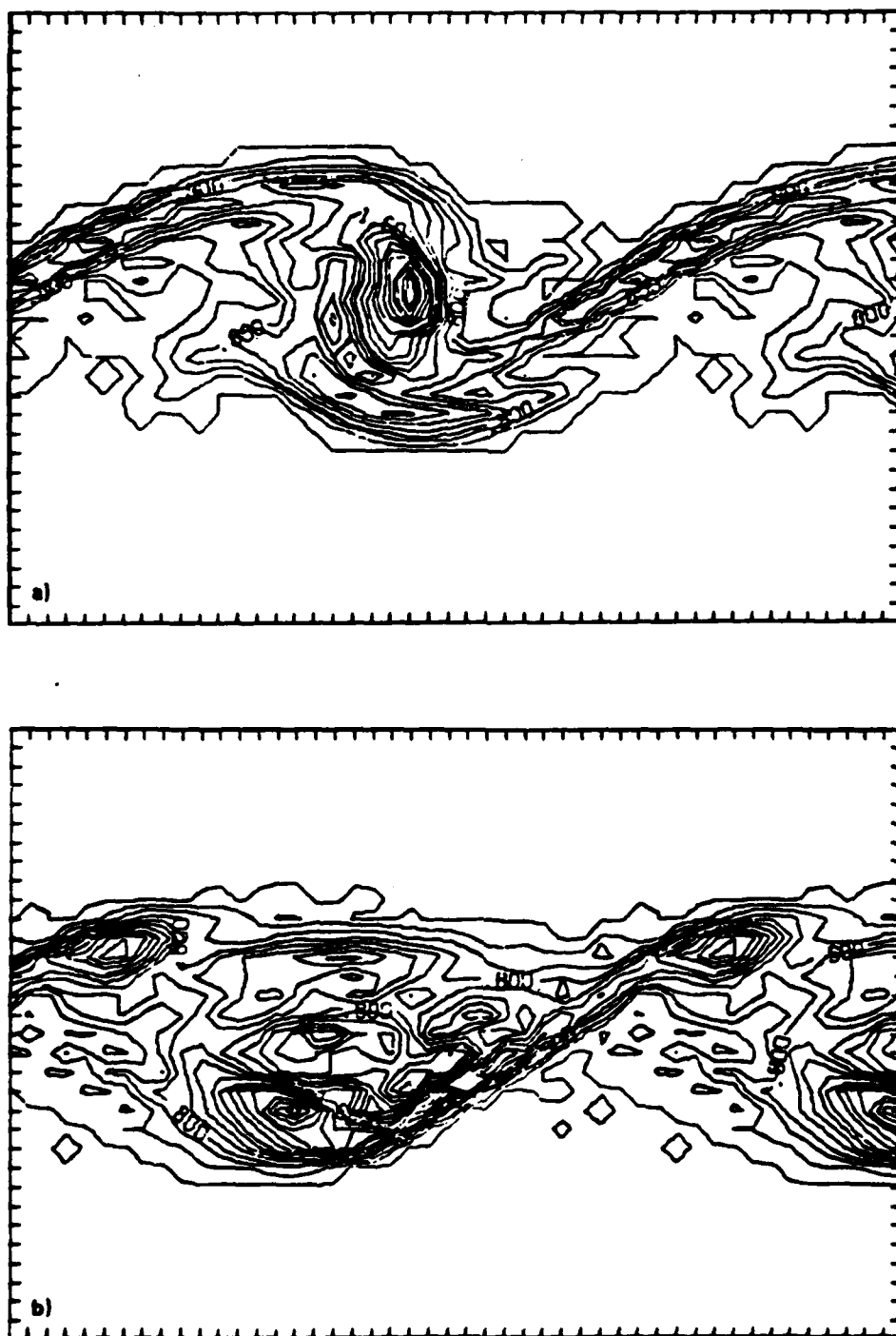
Figure 3 Distribution of the spanwise vorticity component in a turbulent mixing layer as viewed in the spanwise direction. The distribution is shown in two planes separated by half the computational period (from Riley & Metcalfe 1980b).

of turbulence, Deardorff (1970) calculated this flow at a very high Reynolds number using only 6720 grid points. Schumann (1975) and Grotzbach & Schumann (1979) used up to 65,536 grid points, included temperature fluctuations and heat transfer, and considered a range of moderate Reynolds numbers (Re > 10^4), but like Deardorff, they *modeled* the wall-layer dynamics. In these calculations the mean-velocity profile, turbulent intensities, and pressure statistics are in good agreement with the experimental data. Moin & Kim (1982) calculated the channel flow at Re = 13,800 (based on channel half-width δ and centerline velocity), and extended the calculations to the wall using a nonuniform mesh with total of 516,096 grid points. The computed velocity and pressure field was used to study the time-dependent structure of the flow and its relationship to
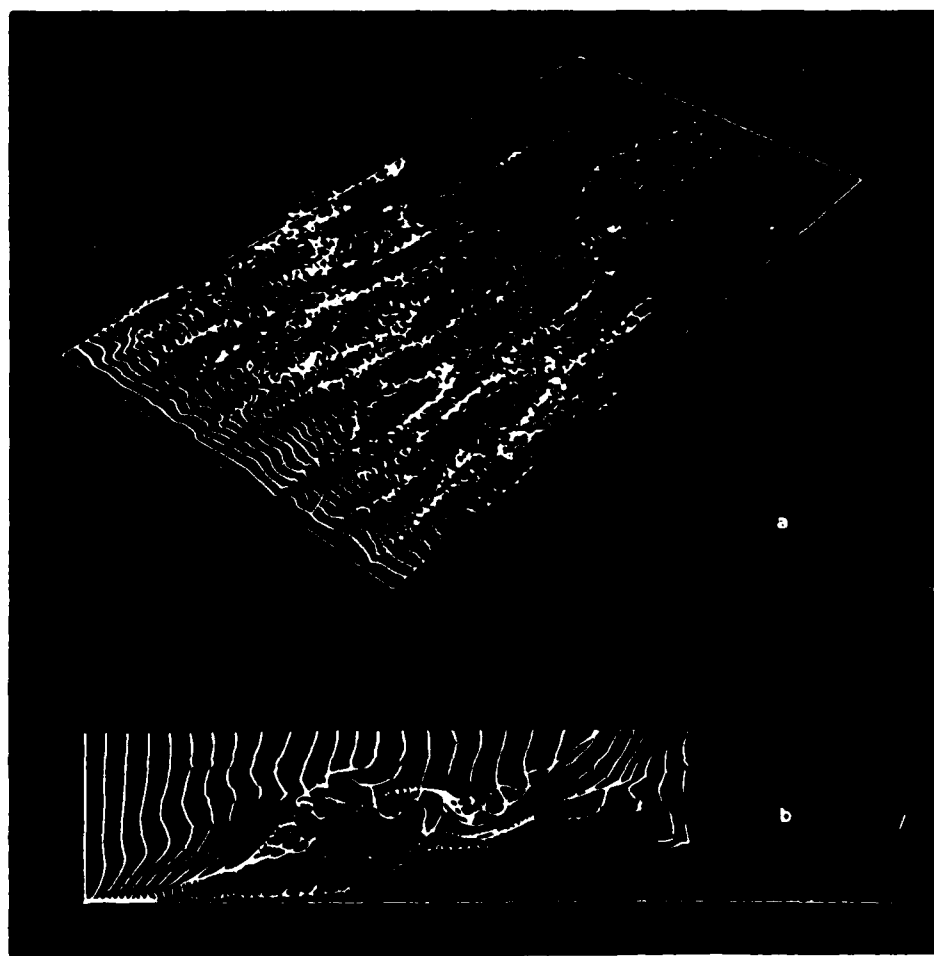

Figure 4 Turbulent channel flow visualized by fluid markers (simulated hydrogen bubbles). (*a*) Markers introduced on a line in the spanwise direction at $y^+ = 6$; (*b*) markers introduced on a line normal to the wall; view extends to $y^+ = 240$ (from data of Moin & Kim 1982).

various flow statistics (including those appearing in the time-averaged Reynolds-stress equations). The detailed flow field was analyzed with contour plots of the instantaneous velocity, pressure, and vorticity fluctuations; with higher-order statistical correlations; and with tracking of passive particles in the flow. In particular, a motion picture was made simulating hydrogen-bubble flow-visualization experiments (see Kim et al. 1971; Kline et al. 1967). In Figure 4 two typical frames from this film show the paths of bubbles generated near the wall ($y^+ \simeq 6$) along a line in the spanwise direction and of bubbles generated along a line normal to the channel wall. Various distinct flow features, including the wall-layer streaks (Figure 4a), and the formation of profiles with multiple inflection points and ejection of fluid from the wall region (Figure 4b), are in accordance with laboratory observations.

The contours of wall-pressure fluctuations from the turbulent channel flow simulations of Grotzbach & Schumann (1979) are shown in Figure 5. In agreement with experimental measurements (Bull 1967, Willmarth 1975), the large-scale pressure fluctuations are correlated at considerably greater distances in the lateral direction than they are in the mean-flow direction. This feature is reproduced in the calculations of Moin & Kim (1982), where localized regions of high pressure intensity are also observed. The two-point pressure correlations of Moin & Kim (1982) indicate that the spanwise elongation of pressure eddies persists across the entire channel. Figure 6 shows the two-point velocity and pressure correlations in the vicinity of the wall ($y/\delta = 0.06$, $y^+ = 38$). The pressure correlation is negative for large streamwise separations but is always positive for
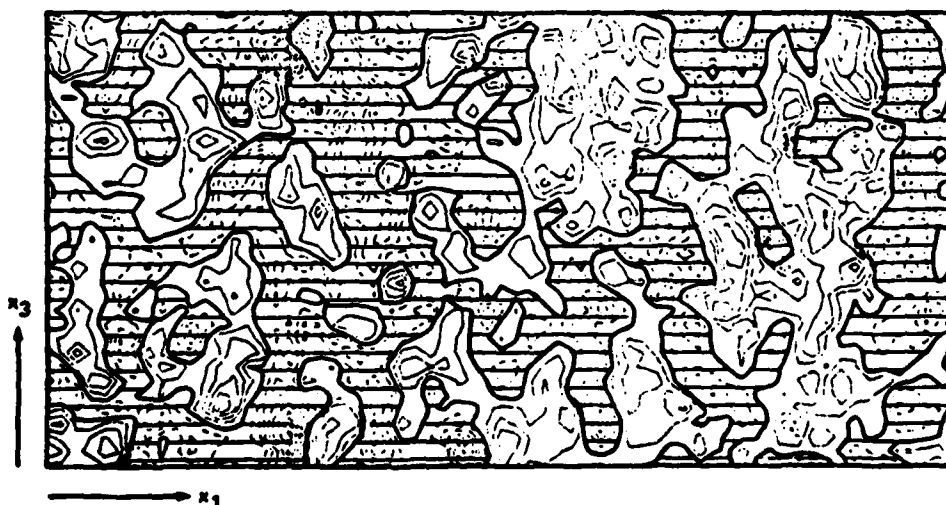

Figure 5 Pressure distribution at the wall in turbulent channel flow (from Grotzbach & Schumann 1979).
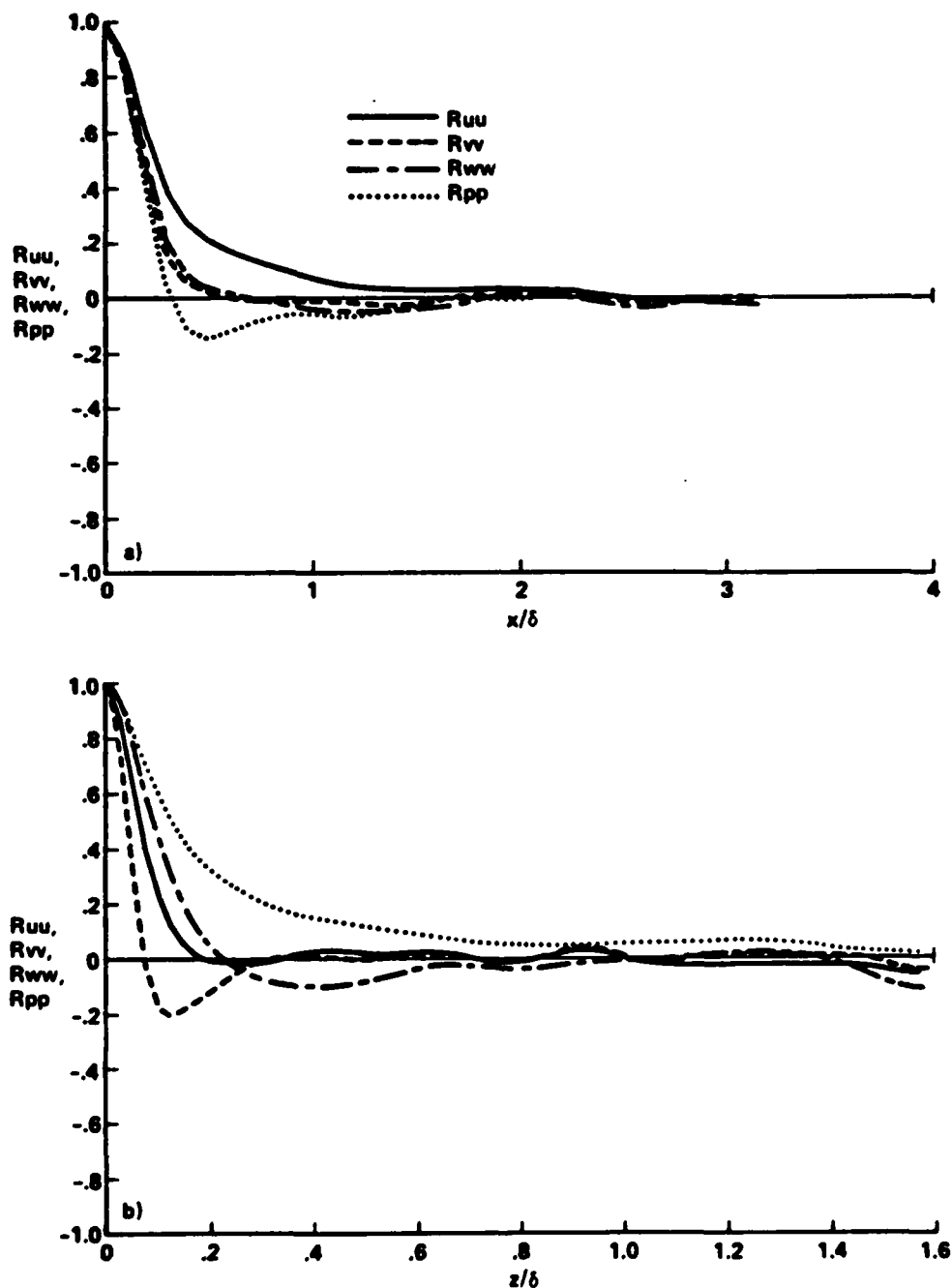
Figure 6 Two-point correlations of pressure and velocity near the wall ($y^+ = 38$) in turbulent channel flow. (*a*) Points separated in streamwise direction; (*b*) points separated in spanwise direction (from data of Moin & Kim 1982).

spanwise separations. The same characteristics are exhibited by experimentally measured wall pressure correlations (Bull 1967). Thus, the fluctuating pressure gradients driving the flow are stronger in the streamwise direction than in the spanwise direction. In the vicinity of the wall the pressure fluctuations are correlated over larger lateral distances than are the velocity components, but in the streamwise direction it is the velocity fluctuations (particularly the streamwise component) that are correlated over larger distances.

Recently, Kim (1983) has further studied the spatial structure of the wall layer by applying a conditional sampling technique to the "data" generated by Moin & Kim (1982). Figure 7 shows the signatures of the pressure and streamwise velocity component, during a "bursting event," obtained using a variant of the VITA conditional sampling technique of Blackwelder & Kaplan (1976). The velocity signatures are remarkably similar to the experimental results. The pressure signatures (which can be obtained experimentally only at the walls) indicate localized peaks during the detected bursting event, with adverse pressure gradient associated with flow deceleration. The pressure signature persists at significantly larger
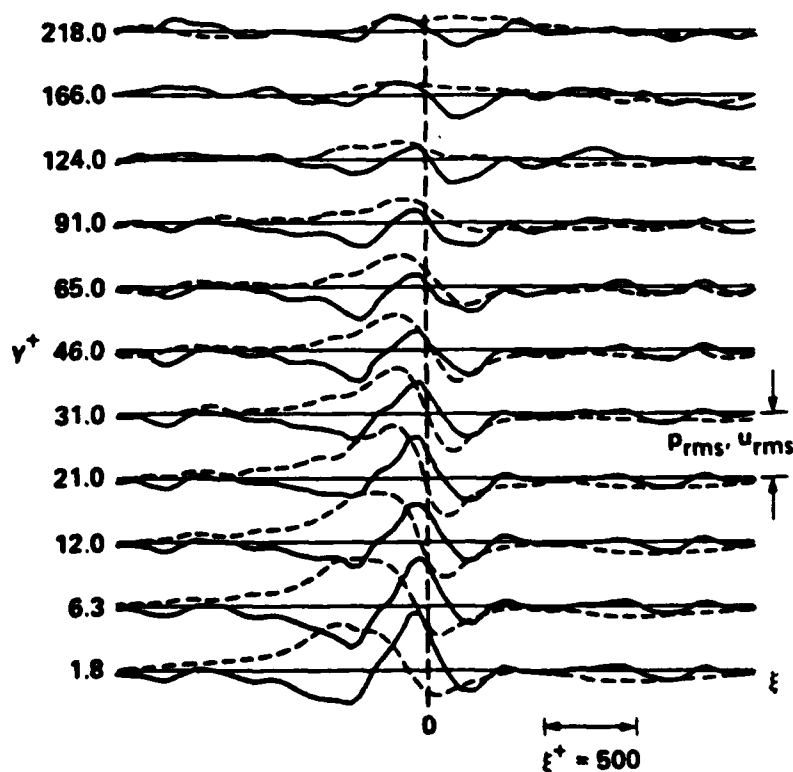

Figure 7 Pressure and velocity signatures of the "bursting event" near the wall in turbulent channel flow. ----- streamwise velocity ; ——— pressure (from Kim 1983).

distances normal to the wall than does the velocity signature; this suggests that the fluctuating pressure gradient driving the wall layer is imposed by the outer flow. The conditionally averaged transverse velocity components and streamwise vorticity component, displayed in planes normal to the flow direction, show a distinct pair of counter-rotating vortical structures associated with the bursting process.

In addition to the fundamental studies outlined above, LES has also been used in practical engineering applications, where it can be more cost effective than the multiple transport equation statistical models (Schumann et al. 1980). For example, in a problem related to nuclear-reactor safety, Grotzbach (1979) used a very-coarse-grid (16 × 16 × 8) LES to investigate the effect of buoyancy on flow mixing in the downcomer of a reactor. He found that buoyancy enhances mixing of the entering hot and cold fluid streams and prevents a "hot chimney" from developing along the length of downcomer adjacent to the reactor core. These results were later confirmed by experimental measurements. LES appears to be the only viable predictive computational tool in applications that involve aerodynamic noise, reduction of turbulent skin friction (for example, flow over compliant boundaries), and other applications in which the details of turbulence dynamics play a dominant role.

7. SUMMARY

Numerical simulation has become a viable complement to experiment in both fundamental and applied turbulence research. Its growing popularity reflects both its promise of realistic answers to a difficult problem and the continuing rapid decline in computing costs. We expect this trend to continue. In addition to the advances in computer capacity of the last decade, less easily measured progress has been made in simulation technique and in the utilization of simulation results. A notable development in numerical algorithms has been the use of spectral methods for direct simulations in simple geometries. This method is not very attractive at present for complex LES calculations involving mesh mapping and implicit time advancement. The premise of LES, that turbulence calculations can be closed more easily by truncating scales of motion rather than statistical moments, is supported by results, especially those in wall-bounded flows. But the hope that very simple eddy-viscosity models would be sufficient has not proved correct for the anisotropic SGS stresses caused by high mean field gradients, at least with a reasonable number of mesh points. Anisotropic meshes, which cause ambiguity in the definition of SGS length scales, and moderate Reynolds numbers, at which the roles of the various scales overlap, introduce additional modeling difficulties. The

decomposition of SGS stress into mean and fluctuations, which essentially models separately the SGS energy transfer from the mean flow and that from the remainder of the resolved scales, provides a workable closure for the wall-bounded cases reported. Despite the ad hoc nature of the model, it demonstrates the ability of an LES to base the SGS model on subsets of the resolved set of scales. The explicit calculation of the Leonard and "cross" terms, and the related modeling ideas of Bardina et al. (1980), also directly utilize more information from the resolved scales to reduce model error.

The nature of the flow near walls requires the expensive resolution of very small scales. The cost of resolution can be reduced by embedding a fine mesh only near the wall. However, the scale disparity between "wall" and "wake" layers, the presence of the overlap "log" layer, and the known form of the organized eddies near the wall strongly suggest that in some practical applications the wall layer can be replaced by a boundary condition for the wake layer that is imposed in the log layer. This situation is analogous to the separation at high Reynolds number of the energy-containing scales and the dissipative scales by an inertial range, and we certainly believe closure is possible in the inertial range in that case.

Inflow and outflow boundary conditions present a major obstacle in the calculation of complex engineering flows. In self-similar cases (wakes, jets, mixing layers, etc.) the use of periodic boundary conditions in the appropriate similarity coordinates seems natural, but in the more general case it will be necessary to measure the sensitivity of computed values to the inflow and outflow conditions used.

The future of turbulence simulation appears bright indeed. While there remains much work to be done on simulation technique, modeling, and numerical methods, we have already reached the point of being able to generate more information than we are able to digest. One can imagine in the near future a researcher at a graphics terminal with access to computed turbulent flow fields of high resolution. He will be able to display any desired quantity computed from the field (for example, statistical averages or three-dimensional visualizations of fluid motion and eddy structure). The computer can answer any question about the fields it holds, and the researcher can devote his time to the really difficult effort of finding the right question to ask. The experimentalist must arrange his experiment and gather the specific data needed to answer his questions; if these answers suggest other questions, the experiment must frequently be rerun to collect new data. The use of stored simulation results places fewer constraints on the questions that can be answered, and allows rapid interactive display of results. An experimentalist with access to such a data base would be able to evaluate the choices of data to be taken from the experiment; for example, he could tune a conditional sampling strategy to capture more precisely the

events of interest. A person developing turbulence models could use the data base to evaluate proposed models. Furthermore, the flow-field data base can be shared by other researchers who do not have the computer power required to generate the fields, but do have enough power to probe them. The development of hardware and software tools for interactive probing of simulation results, the availability of the computed flow fields (in computer-readable form), and the advancement in computer capacity will ultimately determine the degree to which simulation enhances our understanding and ability to control turbulence.

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